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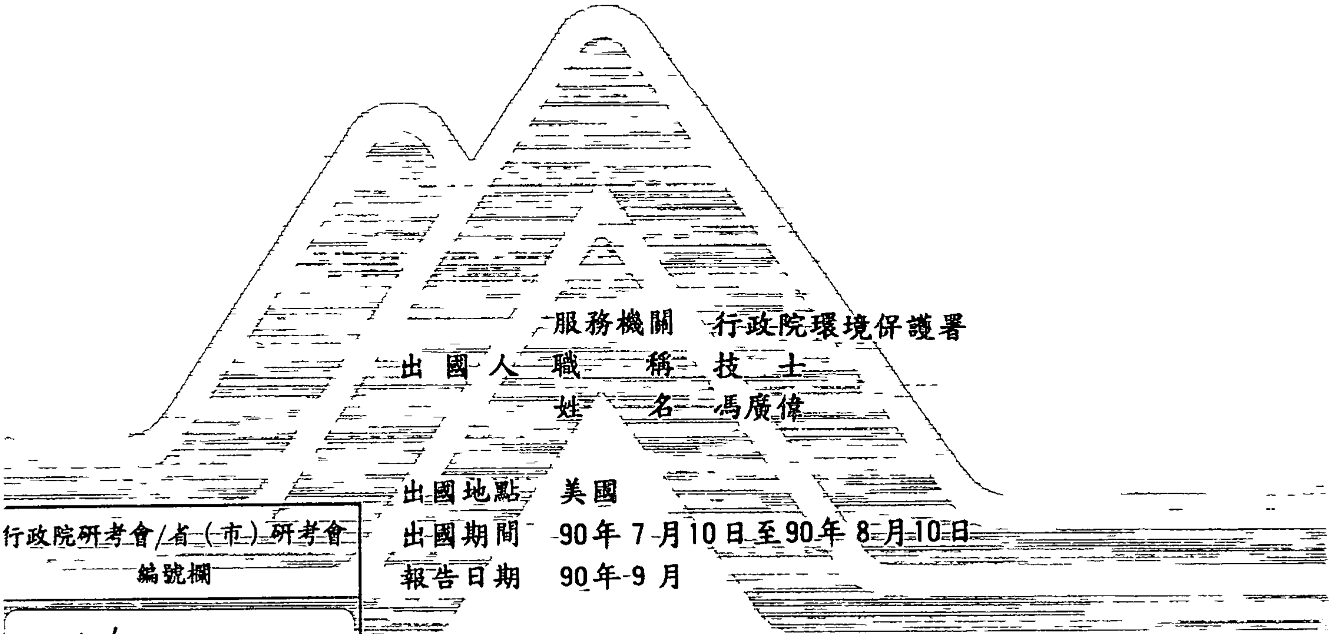
（出國類別　研習　）

集水區總量管制模式應用
出國報告



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關鍵詞 總量管制模式應用

內容摘要 模式在總量管制爲一重要角色，在1972年美國頒布清水法，總量管制在美國EPA、州政府 都積極展開，模式可預測及評估總量管制削減方式，期使水質清澈，而我國目前尚未施行總量管制制度，此次研習希望能汲取美國集水區總量管制模式應用，作爲未來努力之借鏡。

集水區總量管制模式應用

目　錄

表目錄

圖目錄

摘　　要

近十五年來，模式應用在總量管制之河川、湖泊水質污染模式(Water Quality Models)的發展及運用突飛猛進，主要原因是一些工業先進國家急需保護環境，解決水污染問題，加上電腦技術的進步及與水污染相關之科學如生物學、化學、生態學、作業研究（Operations Research）、數值方法(Numerical Methods）的快速進展。

一般而言，模式（Models）可被區分為敘述模式(Descriptive Models)、物理模式（Physical Models）及數學模式（Mathematical Models）。數學模式是利用數學方法來描述物理系統(Physical System)，通常是用數學方程式來表示系統參數（System Parameters）與輸入變數、輸出變數(Input and Output Variables)之間的關係。這些方程式可能是一個簡單的式子，也可能是必需用電腦來解的數千個複雜的聯立方程式。目前，美國模式應用在總量管制也日趨增多，從美國法令清水法(Clean Water Ac)1972頒定總量管制立法後，總量管制在美國EPA、州政府及縣政府正積極展開，而模式也在總量管制應用上擔任重要不可或缺角色，期望使水質符合水體水質標準而更加清澈。

考察及訓練內容

一、集水區總量管制之介紹

現行的水污染防治法相關法令中，作為取締工廠排放污染物之依據的放流水標準，係採濃度標準來管制。其對象是針對工廠、礦場或經中央主管機關指定之事業，對其排放廢水之排放口所採取的一種管制污染方法。執行時則以濃度多少ppm（parts per million百萬分之一or mg/l）來進行判定，為的是防止高濃度的工廠事業，廢水經由排放口排入到河川、海岸或湖泊任何水體而使水體環境惡化。

大部份工廠作業人員甚至業主本身具有環境保育觀念並不多見。一般都認為將工廠製成產品所產生的廢水、廢棄物，移至工廠之外就沒事了。也就是認為將廢水排放到廠外的河川、湖泊、海岸，將廢棄物由垃圾清潔人員收走或傾倒在廠外的空地就算是排除工廠內部污染的問題了，而不願花額外的經費在處理工作上。然而在放流水標準方面，水污染防治法中有明文規定 排放廢水濃度不得超過放流水標準。由於廠商負責人不願花經費在處理污染設備上。因此，一旦排放廢水濃度超過放流水標準時就運用稀釋原理，注入大量的水來稀釋，使其濃度降低，以符合放流水標準免遭取締受罰。造成大部份工廠超抽地下水來稀釋，以降低濃度只為符合放流水濃度標準之要求，卻引發另一環境問題－地層下陷及海水入侵等現象。雖然加入大量的水可以降低其濃度，

但是根據物質平衡（Mass balance）的觀念，其排放廢水濃度降低而總水量增加其所排放的污染物總量卻沒有減少。故總量管制發展為水污染管制未來重要課題。

隨工商業蓬勃發展，事業廢水顯著增加，部分河川的水質在傳統的放流水標準管制下，並未見改善，故應於水污法中引進總量管制之觀念，其乃是以水體水質為主要考量，藉由總量的管制使污染量能低於河川涵容能力，俾有效地改善水質。

總量管制可以下式簡單表示

TMDL=WLAs + LAs + MOS

WLAs　表示點源之分配量（Waste Loads Allocation）

LAs　表示非點源之分配量（Loads Allocation）

MOS　表示邊際安全係數（Margin of Safety）

TMDL　TMDL＝LC(Loading Capacity)表示水體最大之負荷量。

由於分配量影響人民權益極大，需要有精密之計算工具，才能令污染者心服口服。因此，近二十年來，美國大力推廣總量管制相關模式，從簡單之篩選模式至複雜之多元模式，以供各種不同流域或水體之規劃使用。

二、集水區總量管制對象訂立及排序

總量管制實施時，首先需決定那些區域需納入管制，此項工作是確立實施流程後首需進行的工作，初期實施時，若完全依法令規定進行初步篩選可能需納入的水體過多，如此，所需花費在

進行相關分析、擬定計畫書、審查及修正等工作的經費、人力及時間均不符合效益，且不易得到預期成效，故初期建議在篩選時至多宣告一至三個管制候選區為原則。而水體方面，因工商業的急速發展，很多水體水域的污染防治均已到了不容忽視的地步，河川、水庫與湖泊、海岸及地下水均在此之列，然考量現況，部份水體及水域實行總量管制之可行性較低，如海域及地下水等，較難評估，且管制制度尚未成熟，短期內恐難實施總量管制。因此初期建議以河川、水庫與湖泊及港灣為主要對象。

(一)總量管制候選水體對象依據

符合以下任何一項之水體得列入總量管制候選水體。

1 需特予保護且水質未達水質目標或水質正惡化中之水體。

2 污染物曾在近三年內造成環境危害事件者。

3 水質不符合目標水質20%者。

4 水質連續兩年持續惡化者。

5 污染量推估超過預估涵容能力30%。

但在沒有下水道的地區，若削減事業污水之點源污染量仍無法達到顯著地改善水質時，暫不宜列入。

(二)候選水體對象背景資料

1 水體及其上游之流域示意圖。

2 水體上下游邊界水質表。

3 水體水質目標（近、中、長程)。

4 水體污染源（含點源及非點源）分佈及污染量推估。

5 水體涵容能力分析（含流量、水質及流達率分析）。

6 水體相關計劃執行情形及其成效或影響。

7 水體污染過去兩年之管制稽查報告。

8 簡易水質模式報告及詳細模式所需資料與資料缺乏之程度。

(三)總量管制候選區域對象之排序

候選區選擇有二種方式一為ELECTRE METHOD，此法以超越關係以及最小優勢方案並藉由淘汰較差方案，來縮小所要選取的方案數目。另一法為層級分析法AHP法利用問卷調查方式建立各替代方案間的成對比較，以向量代表各替代方案的優先順序，作為各方案間的評估結果。

AHP與ELECTRE兩種方式比較因AHP必需透過問卷調查來評估受訪者較無耐心填寫故較不客觀。而ELECTRE Method評估過程較AHP法客觀，權重建立後不需再經過冗長的問卷即可得到結果，資料的輸入也不似AHP法般的繁瑣，確實適合做為將來區位篩選的模式。

三、集水區總量管制點源及非點源探討

總量管制對象主要可分為點源及非點源污染管制二部份，以下就此二部份，分別說明。

點源污染總量管制

點源污染如事業廢水、家廢污水等，傳統上是以濃度標準進

行管制，濃度管制法簡單易懂，此法假設低濃度較不易造成重大水質影響，當污染源少時，此假設可成立，然而當污染源及廢水量增加時，即使在低濃度的狀況下，河川水質仍可能會顯著地受到影響。加上一些不守法的排放者以抽地下水稀釋廢水，而不實際處理廢水，如此更加速水體水質之惡化。總量管制之觀念於是引進新的水污法中，希望藉由總量的管制使污染排放量能低於河川涵容能力，使水質能有效地改善。

至於應用於估算涵容能力之水質模式，目前美國已有成熟之模式可用，然而每一個模式均有其限制，所得結果之精確性亦可能因不同使用者而有不同程度之差異。而涵容能力之計算及總量削減與分配之影響評估在總量管制中甚為重要，對模擬結果精確度之要求較一般水污染防治規劃為高，因此發展一套針對模式品質保證QA/QC、採樣規範、及流達率估算之指導與評估程序亦甚為重要。QA/QC可保證模式之模擬品質，採樣規範可協助當在進行河川水質監測採樣工作時，能配合模式需要取得較有效的數據，以供模式驗證。而污染流達率資料在總量估算上甚為重要，亦須要有一個規範。另外，設計流量沿用Q75之適用性亦有必要進一步探討。尤其南北兩地河川流量特性不同，加上很多河川上游有水庫存在，水庫操作情形亦影響流量之變化。

非點源污染總量管制

在非點源污染方面，水質保護區及山坡地之開發一直是受爭

議的事件，高爾夫球場之興建、山坡地開發、水庫上游之超限農墾等，已是不容忽視的環保問題，非點源之管制遠較點源污染困難，若未能即早預先防範污染之擴大，未來將需要更多的經費來進行整治。當點源逐漸受到控制，非點源污染在美國國家已變成一項重要工作（USEPA, 1987, 1990）。

目前具體地將非點源污染納入總量管制系統的，以美國較完整，總量管制流程（USEPA, 1976, 1989, 1991），非點源污染主要透過負荷分配（Load Allocation, LA）制度進行管制。因其有較龐大及長時間的人力進行模式發展，已有相當多的模式。故可應用在總量管制上，以使水質改善更加清澈。

四、美國集水區總量管制法令與管制程序

美國在水污染防治的工作上，由聯邦政府環境保護署（US EPA）定出政策性、原則性的法律條文，再由各州政府或地方分署根據母法依照該州或地區的特性，訂定適合該州或地區的施行條例，以有效進行水污染防治的工作。美國對於各種工業污染物總量管制的規定，分別列於各工業分類的放流水限值標準中，EPA訂定一套辦法，廣泛而詳細地調查評估各類工業的各種不同放流限值，適切的將性質相近似的工廠劃分歸類，以規範各類工業污染源的總量排放標準，而更能合理且有效地規範工業污染物的排放。

在美國「聯邦水污染控制法」（Federal Water Pollution Control

Act）中明文規定，任何工廠、事業、或個人將污染物排入水體中，必須領有EPA或經EPA授權之州所發給的「排放許可證」方可排放，即有名的「NPDES」制度。申請「排放許可證」時需擬具放流水監測系統計畫，並依規定提供申請許可證所需資料，如廢水特性、污染物成分、排放污水量及測定方法等。申請書須先送至州政府存檔，30天之內送至區域之EPA許可證審理處（The Regional EPA Permit Section）審理，在審核期間需先擬出一份草案，包括各項管制標準、監測系統設備、以及工作進度要求的草案。州政府在預備發放許可證30天前，需將許可證內容公告週知，此時，也可要求舉辦地區性聽證會。聯邦水污染防制法中規定，只有公告草案並經地方EPA，行政首長核准後，始可發給排放許可證。

美國「NPDES許可證」申請程序，其優點在於主管單位能主動掌握污染排放源所排放之污染物種類，以及所排放之污染負荷量，並依據聯邦水污染防制法的目標之要求減低排放量，擁有排放許可證後即務必遵守規定，否則將會受到刑事處分。透過「NPDES許可證」制度，可對事業單位加以列管，可使主管機關確實掌握有進行生產、操作的工廠數量及排放情形，以防止不利於水體正常使用的情形發生。

然而在新的聯邦水污染控制法中已明定了總量管制條文（FEDERAL Water Pollution Control Art, section 303(d)，文中用

waterquality based control及total mass daily load(TMDL)等名詞），其重要條文如下

1 (a)當水體無法以301(b)(1)(A)及301(b)(1)(B)有效控制其水質在水體標準下時，州政府應界定出這些水域及訂定優先管制的順序。

(b)同上，但以維持水體溫度，避免使魚類或其它野生動物受到傷害而影響生態平衡為主。

(c)州政府應以(a)所列之水域及優先順序，針對各種污染物質計算容許之TMDL，並考慮季節變化及邊際安全性（margin of safety）。

(d)類似(c)，但著重於溫度。

2 當污染物質依304(a)(2)(D)節規定被提出時，在180天內州政府須依第(1)節內容向上級(Administrator)提出總量管制申請計劃，而上級須在30天內回覆是否批准所提之總量計劃。

3 州政府須對所有未列入(1)(A)及(1)(B)中之水體分別依304(a) (2)所列之污染物及熱排水計算TMDL值，同樣地，TMDL之計算須考量季節變化及邊際安全性。

4 對修改排放限制之規定

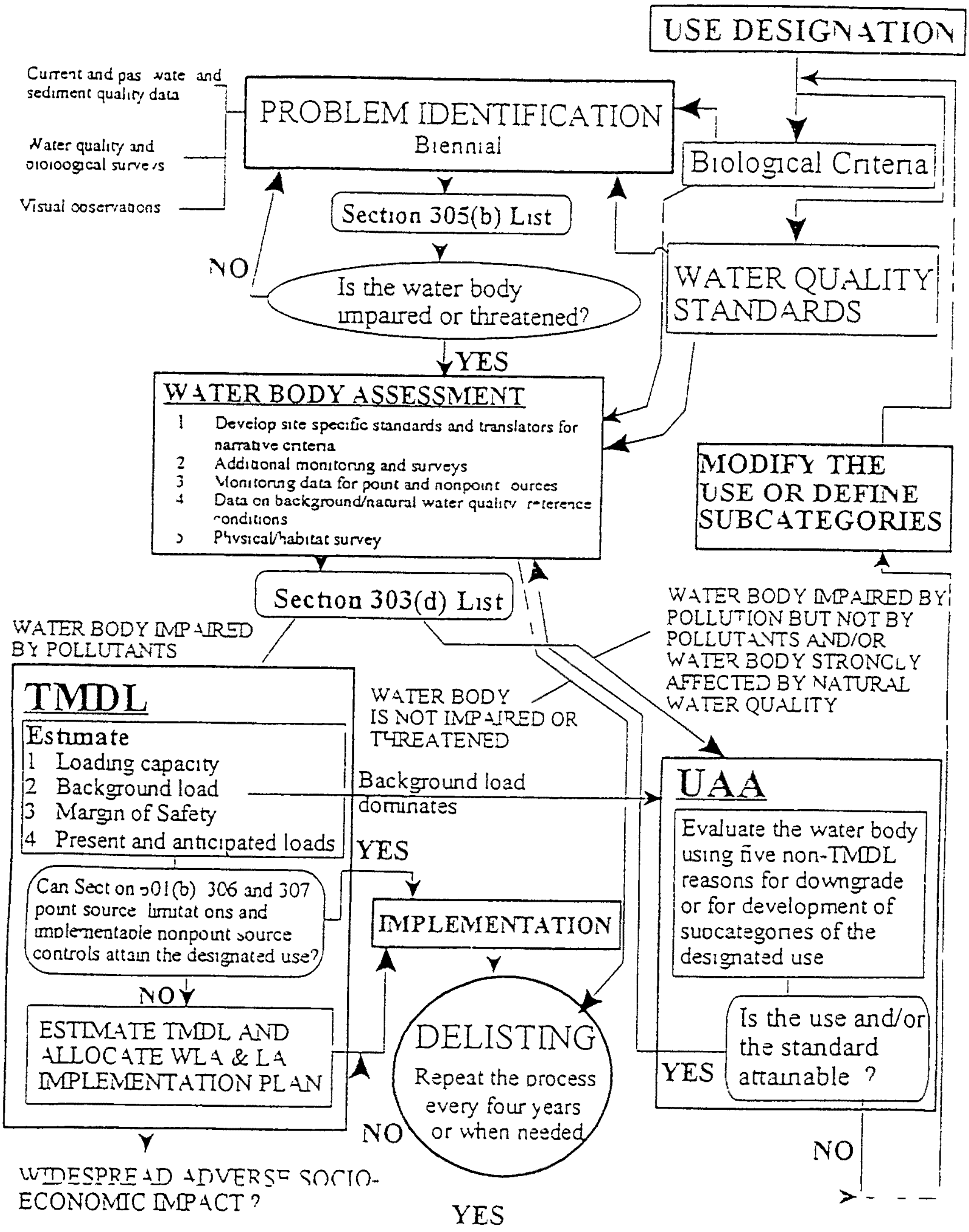
(a)當未達到水體水質標準時　總量管制計劃執行後，任何排放限制之修正只可在以下二種情形下進行(1)所有依TMDL或WLA（waste load allocation）修正之累積影響仍可保證水體

水質標準，(ii)水體用途依法修正時。

(b)當達到水體水質標準時 須在滿足水體水質不變差政策原則（antidegration policy）下，方可進行修改。

圖 1 為美國總量管制程序，首先為確認水質問題，於清水法305(b)列出可疑受損或受威脅之水體後進行水體評估，經由監測資料與水體水質標準比較，若超過水體水質標準則正式列入清水法303(d)正式候選區域，經由總量管制模式作點源削減，非點源削減分配及邊際安全削減分配改善水體，若水質經削減分配後達水體水質標準，則提出候選區域之排除，當候選區排除後，則長期監測該候選區之水質監測，每四年提出檢討修正。

圖1 美國河川集水區總量管制流程圖



五、總量管制分類方式

基本上，若要使整個河川流域之水資源得到最有效的利用，則應該以資源多目標之觀點進行水管理，但是，在環保機關的立場，所關心的是，如何使未受污染的河川保持原貌，以及使已受污染的河川恢復舊有風貌。有其追求的目標與權限，由於至今各國之河川流域管理的單位多以行政區域劃分，無統一的單位加以統籌管理，以致在進行水質管理策略之擬定工作時，多無法也不願意將其他相關目標納入考量。故過去與現在之實際考量與執行上，仍舊多以單目標之最佳化模式來進行水質管理策略之擬定工作，較少將多目標予以納入考量。

一般而言，水質管理之主要目的乃在於決定水質管理策略，以管制流域內各污染源之排放量，期能使河川水體之水質達到特定的水質標準，進而達到水資源保護之目的。過去在水質管理研究領域上，一般多以單目標之最佳化模式，配合最佳化之技巧（多為線性規劃）來進行水質管理策略之擬定工作，只是各種最佳化模式所考慮的目標〔多以廢（污）水處理成本極小〕與限制條件〔河川水質標準與廢（污）水處理效率等限制〕有所不同而已。於所考慮的目標為可排入的污染負荷為最大，限制條件則包括河川水質標準、廢（污）水處理效率、公平性等限制。

而所採用的污染總量分配方法主要以最大污染負荷法、等去除率法、分區等去除率法、分類分區等去除率法及分區等濃度法

等五種方法。上述五種方法概述如下

1 最大污染負荷法　本法之目標在於整個流域可排入水體之污染負荷為最大，但在追求此一目標的同時，除需滿足技術（污染去除效率）與法令（水體分類水質標準）等相關限制條件，此外若因排放濃度低於該處水體水質分類標準之排放口，對於水體而言具有污染稀釋的功效，可不需參與污染總量分配程序，且其餘參與總量分配之排放源，最小去除率之限制源自於放流水標準的規定，而最大去除率則僅要求其處理至水體水質分類標準為止。

2 等去除率法　追求的目標仍是整個流域可排入水體之最大污染負荷，但是，在限制條件裏，除上述之限制條件外，尚需增加各污染源（排入水體者）去除率必須相等之限制條件。換言之，本法旨在將水體之涵容能力平均分攤給所屬各排放者。然而針對前述最大去除率限制以及部份排放源未參與總量分配程序加以考量後，有可能出現各排放源之去除率不等的情形。故與傳統所謂之「等去除率法」相較之下，本計畫所使用的應屬廣義的等去除率法。

3 分區等去除率法　此方法和等去除率法相似，不同點僅在於本法將施行總量管制之流域分為數個區段，而同一區（可能有幾個污染源）污染源之去除率相同，但不同區污染源之去除率並不相同。

4 分類分區等去除率法　此方法和分區等去除率法最大的不同在於本法針對各類分區分別訂定其去除率限制範圍，並依此做為污染總量分配原則。首先除各類分區內之排放源應達成統一之去除率外，若因排放濃度低於該處水體水質分類標準之排放源，對於水體而言具有污染稀釋的功效，則可不需參與污染總量分配程序，且參與總量分配之排放源，去除率最高僅要求至達到水體水質分類標準為止。除此之外，各排放源仍需遵循放流水標準做為個別最小去除率之限制條件，雖然此一限制條件在本案例大部分的情形下應非作用限制式。

5 分區等濃度法　本法亦是將施行總量管制之流域分為數個區域，同一區內之排放源（除前述不需參與總量分配程序及已削減至水體分類水質標準的排放源外）均需去除至相同之排放濃度，而不同分區內之排放源則不需去除至相同濃度。故本法與等去除率法的相異之處僅在於其限制條件為各排放源之排放濃度需相等，而等去除率法則為各排放源之去除率需相等。

六、總量管制模式發展及介紹（含模式分類）

(一)總量管制模式發展

西元1925年Streeter和Phelps二氏研究Ohio River水質後，發表了計算河川BOD-DO的Streeter-Phelps方程式（Streeter and Phelps, 1925），開啟了水質模式的發展與應用。1938年Velz研究發表了表面更新模式（Surface-Renewal Model）（Velz, 1938

），1941年Fair等人研究河川底泥對溶氧之影響（Fair, 1941），1958年O' Connor和Dobbins發表了廣泛被應用的再曝氣半經驗公式（O' Connor and Dobbins 1958），1963年O' Connor利用質量平衡的原理闡述Streeter-Phelps方程式（O' Connor 1963），至此水質模式的發展具備理論基礎。

1960年以後，水質模式之發展更為蓬勃，Thomann(1964)、Dobbins(1964)、O' Connor (1967)及Di Toro(1968) 等學者的努力研究，對於光合作用、底泥耗氧、氮系統及植物呼吸作用的考慮，使水質模式可應用於更複雜的系統，同時進一步使水質模擬之結果，更能確實反應出實際水質狀況。至目前為止，水質模式之研究方向與應用，已著眼於湖泊的優養問題及毒性物質對水質的影響。

(二)總量管制模式介紹

1 使用模式的觀念

一般人往往誤解使用模式的目的，因而有必要先作一說明，在使用及評估模式時，一般人往往先問模式準不準，雖然，模式的準確性甚為重要，但使用模式的更重要目的是希望藉由模式了解所面對問題的可能變化範圍，即使模式針對某一特定時間狀況及區域求得非常準確的結果，但對不同時間、狀況會產生甚異常結果時，則如此的模式並沒有多大用處。更須注意的是，一個好模式可能因使用者對模式及參數

的不了解，而設定錯誤的參數值，雖在表面上符合率定的實測值，但實際用於推測時，則與合理範圍相去甚遠。另外，有些模式雖不能準確模擬實況，但卻可用於比較不同方案之優劣。因而使用模式首先須確定分析的目的是什麼及了解模式的適用性，進而選定適當地模式，然後了解模式的參數值，收集、分析及設定參數，之後才進行率定與驗證的工作。且這樣地工作若能長期地做下去，在逐年的修正下，則一定會找到或發展出適用於某區域的模式。

非點源污染之模擬比點源困難度高很多，加上非點源污染評估往往不易取得大量的資料來驗證，尤其是國內流域性的監測網尚未建立，資料往往不足，雖然國外有不少依地區特性（physical based）模式可用，不必率定，但其所用的參數表經常不太適用於國內。使得模式模擬結果與實際值差異頗大。

雖然有上述之困難，但不表示應停用模式分析，反而應儘早使用模式分析，逐漸建立參數，才能建立適當模式，即使在美國先進國家，一個模式也是歷經數年的測試修正才廣為分析者使用。

2 模式分類

(1)流域負荷模式　又分以下三種模式

①簡易模式　資料需求量少，可在短時間評估出需注意的

區域。往往是在時間及經費不足的情形下使用，這些方法只分析大區域的整體變化，對局部變化的影響不太適用。這些方法是架構在長期應用所得的經驗公式下，若能長期修正，對某特定區域之總體平均污染量之評估不致相去太遠。此種方法通常用於算年平均或單場暴雨的污染量。

②中度模式　可評估不同污染源之影響及衝擊，有些可與地理資訊系統相結合，但不少模式採用一些簡化的公式，使誤差有時會很大。主要是用於找出一個大區域中的重點區域或用於初步評估一些非點源污染削減最佳計畫(BMP)的效果。有些中度模式可分析季節性的變化，通常亦可分析不同土地利用的影響，不過此種分析往往需先有一些經驗公式可用。因而通常需要一些區域性的資料。

③評細模式　此種模式不只是分析整體性變化，若有足夠及適當的資料，可分析流域中任一區域的水質及水流等資料。但因較複雜，所需的資料較多及需花較多時間，且往往需由專家來進行模擬工作。

(2)現場負荷模式

對總量管制之點源與非點源皆有探討，提供微尺寸管制決策參考依據。

(3)承受水體模式　又分以下幾種模式

①水動力模式　模式如RIVMOO, DYNHYD5 EFDC和CH3D-WES可以單獨使用或外部連接水質模式，如WASP5和CE-QUAL-ICM等模式。其它模式則是內部連接水質及毒性模擬計畫如QUAL-RIVI和CE-QUAL-W2，此種模式係以時間變化描述水之傳輸。

②水質模式　模擬化學和生物程序根據內部和外部輸入資料和反應。其中優養化模式包括模擬生物輸入資料，營養物、藻類生長在河川湖、水池及感潮河段地段。此水質模式包括穩態水質模式（Steady-State models）及動態水質模式（Dynamic water-Quality models）。其中穩態水質模式QUAL2E及動態水質模式WASPS和HSPF最常被USE PA使用。

③混合層模式　混合層模式被定義為近場模式，他們被限制在廢水處理場排放污染混合區域，此種模式較少被使用。

(4)整合模式系統　此種模式為總合數種模式串聯使用，可增加模式功能，但較複雜，此種模式需有4種功能配套較易使用①容易使用②不同模式可以彼此連结③可以連结模式到資料庫④所用模组（modules）讓使用者很易去選擇特殊分析。其中BASINS最常被USEPA使用，此模式為由

QUALIE和HSPF兩種模式共同組成，另現民間開發WARMF也較常使用。

圖２為總量管制模式分類表，表1至表5為模式之名稱及一些因子作比較。

Figure 2 Overview of Models

Watershed-scale loading Models
(Section 2 3)

Simple Methods
- EPA Screening
- Simple Method
- Regression Method
- SLOSS-PHOSPH
- Watershed
- Federal Highway Aministration Model
- Watershed Management Model

Mid-Range Models
- SITEMAP
- GWLF
- Urban Catchment Model
- Automated Q-ILLUDAS
- AGNPS
- SLAMM

Detailed Models
- STORM
- ANSWERS
- DR3M-QUAL
- SWRRBWQ
- SWMM
- HSPF

Field-Scale Loading Models
(Section 2 4)
- CREAM/GLEAMS
- Opus
- WEPP

Integrated Modeling Systems
(Section 2 6)
- PC-VIRGIS
- WSTT
- LWMM
- GISPLM
- BASINS

Receiving Water Models
(Section 2 5)

Hydrodynamic Models
- RIVMOD-H
- DYNHYD 5
- EFDC
- CH3D-WES

Steady-State Models
- EPA Screening Procedures
- EUTROMOD
- PHOSMOD
- BATHTUB
- QUAL2E
- EXAMS II
- TOXMOD
- SMPTOX3
- Tidal Prism Model
- DECAL

Dynamic Water-Quality Models
- DYNTOX
- WASPS
- CE-QUAL-RIV1
- CE-QUAL-W2
- CE-QUAL-ICM
- HSPF

Mixing Zone Models
- CORMIX
- PLUME

Table1 Evaluation of Model Capabilities-Simple Models

Criteria		EPA Screening [1]	Simple Method	Regression Method	SLOSS-PHOSPH [2]	Watershed	FHWA	WMM
Land Uses	Urban	○	◐	◐	-	◐	○[3]	●
	Rural	◐	-	○	◐	◐	○	●
	Point Sources	-	-	-	-	○	-	○
Time Scale	Annual	●	●	●	●	●	●	●
	Single Event	○	○	○	-	-	○	-
	Continuous	-	-	-	-	-	-	-
Hydrology	Runoff	-[4]	◐	-	-	-	○	○
	Baseflow	-	-	-	-	-	-	○
Pollutant Loading	Sediment	◐	◐	◐	◐	◐	-	-
	Nutrients	◐	◐	◐	◐	◐	◐	◐
	Others	○	◐	◐	-	◐	◐	◐
Pollutant Routing	Transport	-	-	-	-	-	-	-
	Transformation	-	-	-	-	-	-	○
Model Output	Statistics	-	-	-	-	◐	○	○
	Graphics	-	-	-	-	◐	-	○
	Format Options	-	-	-	-	◐	-	○
Input Data	Requirements	○	○	○	○	○	○	○
	Calibration	-	-	-	○	◐	-	◐
	Default Data	●	●	◐	◐	○	◐	◐
	User Interface	-	-	-	-	◐	○	◐
BMPs	Evaluation	○	○	-	○	◐	◐	◐
	Design Criteria	-	-	-	-	-	-	-
Documentation		●	●	●	●	●	●	◐

1 Not a computer program
2 Coupled with GIS
3 Highway drainage basins
4 Extended versions recommend use of SCS-curve number method for runoff estimation

● High ◐ Medium ○ Low - Not incorporated

Table 2 Evaluation of Model Capabilities—Mid-Range Models

Criteria		SITEMAP	GWLF	P8-UCM	Auto-QI	AGNPS	SLAMM
Land Uses	Urban	●	●	●	●	-	●
	Rural	●	●	-	-	●	-
	Point Sources	◒	◒	●	-	●	●
Time Scale	Annual	-	-	-	-	-	-
	Single Event	○	-	●	-	●	-
	Continuous	●	●	●	●	-	●
Hydrology	Runoff	●	●	●	●	●	●
	Baseflow	○	●	○	○	-	○
Pollutant Loading	Sediment	-	●	●	●	●	●
	Nutrients	●	●	●	●	●	●
	Others	-	-	●	●	-	●
Pollutant Routing	Transport	○	○	○	◒	●	◒
	Transformation	-	-	-	-	-	-
Model Output	Statistics	◒	○	-	-	-	○
	Graphics	◒	◒	●	-	●	○
	Format Options	●	●	●	○	●	●
Input Data	Requirements	◒	◒	◒	◒	◒	◒
	Calibration	○	○	○	◒	○	◒
	Default Data	●	●	◒	○	◒	◒
	User Interface	●	●	●	◒	◒	●
BMPs	Evaluation	○	○	●	◒	◒	◒
	Design Criteria	-	-	●	◒	◒	○
Documentation		●	●	●	◒	●	◒

● High ◒ Medium ○ Low - Not Incorporated

Table 3 Evaluation of Model Capabilities—Detailed Models

Criteria		STORM	ANSWERS	DR3M-QUAL	SWRRBWQ/SWAT	SWMM	HSPF
Land Uses	Urban	●	-	●	○	●	●
	Rural	-	●	-	●	○	●
	Point Sources	●	-	●	●	●	●
Time Scale	Annual	-	-	-	-	-	-
	Single Event	○	●	○	○	●	●
	Continuous	●	-	●	●	●	●
Hydrology	Runoff	●	●	●	●	●	●
	Baseflow	○	-	○	●	●	●
Pollutant Loading	Sediment	●	●	●	●	●	●
	Nutrients	●	●	●	●	●	●
	Others	●	-	-	●	●	●
Pollutant Routing	Transport	-	◒	●	●	○	●
	Transformation	-	-	-	-	○	●
Model Output	Statistics	○	-	●	●	●	●
	Graphics	-	-	◒	◒	○	○
	Format Options	●	●	●	●	●	●
Input Data	Requirements	◒	●	●	◒	●	●
	Calibration	○	○	◒	◒	●	●
	Default Data	◒	○	●	●	◒	◒
	User Interface	●	-	◒	●	●	-
BMPs	Evaluation	◒	◒	●	◒	●	●
	Design Criteria	◒	◒	◒	-	●	●
Documentation		●	◒	◒	●	●	●

● High ◒ Medium ○ Low - Not Incorporated

Table 4 Evaluation of Capabilities—Hydrodynamic models

	Externally Coupled Models				Internally Coupled Models		
	RIVMOD	DYNHYD 5	FEDC	CH3D-WES	CE-QUAL-RIV 1	CE-QUAL-W2	HSPF
Waterbody Type							
Rivers/Streams	●	●	●	●	●	●	●
Lakes/Reservoirs	○	○	●	●	○	●	○
Dimension	○	◒	●	●			
1-D	●	●	●	●	●	●	●
2-D	-	-	●	●	-	●	-
3-D	-	-	●	●	-	-	-
Input Data Requirements							
Requirements	○	○	●	●	○	◒	◒
Calibration	●	●	●	●	●	●	●
Grid generation/Interface	-	-	●		-	-	-
Output Data							
Format options	●	●	●	○	●	●	●
Graphics	○	◒	○	○	○	○	○
Hydrologic Structure Simulation	●	○	●	●	●	●	◒
Expertise Required for Application	○	○	●	●		◒	◒
Documentation	●	●	●	●	●	●	●

● High ◒ Medium ○ Low - Not Incorporated

Table 5 Evaluation of Capabilities—Steady-state water quality models

	EPA SCREENING	EUTROMOD	PHOSMOD	BATHTUB	QUAL2E	EXAMSII	TOXMOD	SMPTOX4	TPM	DECAL
Waterbody Type										
Rivers/Streams	●	-	-	-	●	●	-	●	-	-
Lakes/Reservoirs	●	●	●	●	○	-	●	-	-	-
Estuaries	●	-	-	-	◒	-	-	-	●	-
Coastal	-	-	-	-	-	-	-	-	-	-
Physical Processes										
Advection	●	-	-	●	●	●	-	●	●	●
Dispersion	●	-	-	●	●	●	-	●	●	●
Particle Fate	○	○	○	○	-	○	○	●	●	●
Eutrophication	●	●	●	●	●	-	-	-	●	-
Chemical Fate	●	-	-	○	○	●	●	●	○	●
Sediment-Water Interactions	○	○	◒	○	○	◒	◒	◒	●	◒
External Loading-Dynamic	●	●	●	●	●	●	●	●	●	●
Internally Calculated NPS Loading	-	●	-	-	-	-	-	-	-	-
User Interface	-	●	●	○	○	●	●	●	-	○
Documentation	●	●	●	●	●	●	●	●	●	●

● High ◒ Medium ○ Low - Not Incorporated

七、總量管制模式篩選及應用

(一)模式選擇準則如下

1 硬體電腦可運用方便性　現今個人電腦強有力的發展，此硬體電腦因素較為不限制之因子，但仍需加以考慮其技術方便性。

2 專業訓練人才有效性　總量管制模式已變得更加方便給使用人運用，但是一個專業有經驗人才或環境工程師，對模式參數發展及關鍵評估模式結果是無價的。

3 總量管制模式應能配合不同計畫長期使用　如果一些未來計畫需要使用一特殊模式，它是有利的一項措施對目前此特殊模式來說，甚至對目前之計畫較不適合，因長遠亦可採行。有時去大力投資一個模式從一個計畫轉化另一計畫使用是有利用節省人力物力的。

4 公司人員模式使用經驗成熟度　公司人員對特殊模式使用熟練度是相當重要的，在這一方面及有暖身期花在模式運用上將可減少使用此模式經費及節省時間。

5 模式受大眾接受程度　如果模式未寬廣使用且為大眾老百姓接受，它是很難去建立信譽及解釋其結果。

6 利益團體共同決議模式為可接受方式　牽涉在此計畫中各種不同利益團體願意接受模式結果，並有幫助完成政策之執行。

(二)模式於總量管制各階段之選擇尺度

確定參數時應使用較低層次模式或不使用模式皆可，在總量管制優選區域排序時使用較低層次至中等層次模式，在發展總量管制之時使用中等層次至較複雜模式，在設計或完成時使用較複雜模式監測及效益評估時應使用中等層次至較複雜模式。

(三)初步模式選擇之考慮

1 一個獨立模式可能是不夠多方面使用　在模式分類討論章節中大部分模式都是獨立使用在某一特殊目的，獨立模式無法解釋所有集水區污染物複雜相互關係。在面對集水區保護環境管理人，主要當務之急，並非不僅是那一個模式要用，而是多少個獨立模式合起來用以支持一集區環境保護工作概念設計。故模式皆合去建立一工作網，以成功模擬污染物隨時間及空間而變之結果是必需的。

2 一個複雜高層次模式能被運用在各種詳細層次　雖然沒有一個模式是理想運用在各方面，但一良好複雜高層次模式如SWMM及HSPF即是很有利應用各種不同之層次，在許多方面與其從一個計畫轉換不同模式到另一計畫，不如一直用一個良好較複雜在各種不同科學和工程應用，所得之結果較更為精確。

(四)集水區總量管制模式應用及選擇

大部分集水區總量管制模式包括三項成分，第1項為水文部分，其為評估從集水區域或次集水區逕流量及河川流量，第2項為侵蝕及沈澱部分可計算被帶到承受水體的沈澱總量，第3項為計算污染負荷之水質，基本之模式功能列於表6 7 8 含土地利用、水文侵蝕及沈澱、污染負荷、污染物質及時間尺度比較。許多簡單模式當模擬污染負荷時來考慮水文過程，當處理都市區域時簡單模式根據統計方法及經驗方法在逕流參數及不透水程度計算逕流數據，外簡單模式較困難以統計方法求得鄉村及農業之該項數據。

詳細模式用較複雜公式模擬逕流及沈澱之輸出參數。水文要素通常包含一組決定方程式去代來水平衡方程式之成分如滲透、蒸發、地下水補注和滲透等。這些模式也用侵蝕和沈澱輸出機械機制作物理之描述如土壤、分離、傳輸及沈澱，污染物先出預測通常根據一小時階段指數衰退功能而產生
這些模式如果缺乏充分數據將會使模式校正困難，在大部分之情況，適當之試驗數據及現場監測是必需的。集水區總量管制模式主要發展為土地利用和土地活動，較少部分模式是評估混合土地之利用。在詳細模式中HSPF似乎是對複雜土地利用功能最多的。SWMM, STORM和DR3M-QUAL主要設計運用在都市地區，而ANSWERS和SWRRB為運用在農業地區。在中度模式中，SITEMAP和GWLF是運用在鄉村和都市集水區，GWLF模式可提供長時期在各種不同時間序列污染負荷

值，如每季每日之污染負荷值，GWLF也許估土地利用型態，點源和水點源負荷水源區之影響。簡單模式一般應用在鄉村和都市概念的關係，其使用特殊或較少數據即可。

集水區總量管制模式輸入及輸出分析資料列於表9、10、11及12。

集水區總量管制模式規劃應用，設計分析及水質影響分析列於表13、14及15。

Table 6　A Descriptive List of Model Components – Simple Methods

Model	Main Land Use	Hydrology	Erosion/ Sediment	Pollutant Load	Pollutants	Time Scale
EPA Screening Procedures	Mixed watershed	N/A	USLE-MUSLE	Loading functions, potency factors	Wide range [1]	Mean annual
The Simple Method	Urban	Runoff coefficient	N/A	Mean concentration	NURP data TSS, P, metals, O&G	Variable (annual, monthly, event)
Regression Method	Urban	N/A	N/A	Regression equations	TSS N, P, COD, metals	Storm event
SLOSS/PHOSP	Rural	N/A	USLE	Loading functions	P	Annual
Watershed	Mixed watershed	N/A	USLE	Unit area loaing	Wide range	Annual
PHWA	Highways	Runoff coefficient, observed data	N/A	Median concentration	TSS, N, P, organics, metals	Storm event
WMM	Mixed watershed	Runoff coefficient	N/A	Event mean concentration	N, P, lead, zinc	Annual

1 Depends on available pollutant parameters and default data

N=nitrogen　O&G=oil and gas　P=phosphorus　TSS=total suspended solids

COD=chemical oxygen demand

Table 7 A Descriptive List of Model Components – Mid-Range Methods

Model	Main Land Use	Hydrology	Erosion/ Sediment	Pollutant Load	Pollutants	Time Scale
SITEMAP	Mixed watershed	SCS curve number	N/A	Runoff concentration	N P	Storm event Continuous
GWLF	Mixed watershed	SCS curve number	Modified USLE	Unit loading rates	N P	Storm event Continuous
P8 UCM	Urban	SCS curve number (modified) TR 20	N/A	Nonlinear accumulation	TSS N P metals	Storm event Continuous
Anto QI	Urban	Water balance	N/A	Accumulation and wash off	Wide Range	Storm event Continuous
AGNPS	Agriculture	SCS curve number	Modified USLE	Potency factors	N P	Storm event
SLAMM	Urban watershed	Small storm based coefficient	N/A	Nonlinear accumulation and wash off	N P COD bacteria, metals	Storm event Continuous

1 Depends on available pollutant parameters and default data
N=nitrogen O&G=oil and gas P=phosphorus TSS=total suspended solids
COD=chemical oxygen demand

Table 8 A Descriptive List of Model Components – Detailed Methods

Model	Main Land Use	Hydrology	Erosion/ Sediment	Pollutant Load	Pollutants	Time Scale
STORM	Urban	Runoff coefficient-SCS curve numbers - Unit hydrograph	USLE	Buildup/wash-off functions	P,N, COD, metals	Continuous
ANSWERS	Agriculture	Distributed storage model	Detachment transport equations	Potency factor (correlation with sediment)	N/A	Storm event
DR3M QUAL	Urban	Surface storage balance kinematic wave method	Related to runoff volume and peak	Buildup/wash-off functions	TSS, N, P, organics, metals	Continuous
SWRRBWQ /SWAT	Agriculture	SCS curve number	Modified USLE	Loading functions	N,P, COD, metals, bacteria	Continuous
SWMM	Urban	Nonlinear reservoir	Modified USLE	Buildup/wash off functions	Wide range[1]	Storm event continuous
HSPF	Mixed watershed	Water balance of land surface and soil processes	Detachment /wash-off equations	Buildup/wash off functions and sub-surface concentrations	Wide range[1]	Storm event continuous

1 Depends on available pollutant parameters and default data
N=nitrogen O&G=oil and gas P=phosphorus TSS=total suspended solids
COD=chemical oxygen demand

Table 9 Input and Output Data - Simple Methods

Models	Main Input Data	Output Information
EPA Screening Procedures	Watershed and land use data Loading factors (default values)	Mean annual sediment and pollutant loads
The Simple Method	Annual rainfall data Land use and imperviousness data Pollutant mean concentration BMP removal efficiencies	Runoff volume and pollutant concentration/load storm or annual
Regression	Mean annual rainfall Mean minimum January temperature Drainage areas and land use Percent imperviousness	Mean annual storm event load and confidence interval
SLOSS/ PHOSPH	Rainfall erosivity factor Soil, crop, topography, and land use data	Mean annual loads of sediment and phosphorus
Watershed	Rainfall erosivity factor Land use and soil parameters Unit loading rates BMP cost information	Mean annual pollutant loads, BMP cost-effectiveness
FHWA	Site and receiving water data Flow and storm event concentrations	Statistics on storm runoff and concentrations, impacts on receiving water
WMM	Land use and soil data Annual precipitation and evaporation Inputs from baseflow and precipitation Event mean concentrations in runoff Reservoir, lake, or stream hydraulic characteristics Removal efficiencies of proposed BMPs	Annual urban and rural pollutant loads from point and nonpoint sources, including septic tanks, load reductions from combined effects of multiple BMPs, in-lake nutrient concentrations as related to trophic state, concentrations of metals

Table 10 Input and Output Data- Mid-Range Models

Models	Main Input Data	Output Information
SITEMAP	Meteorologic and hydrologic data, hourly or daily (maximum one year) Watershed and channel parameters Point sources and pollutant parameters (e.g., decay)	Runoff and nutrient loadings Pollution load allocations
GWLF	Meteorologic and hydrologic data, daily Land use and soil data parameters Nutrient loading rates	Monthly and annual time series of runoff, sediment, and nutrients
P8 UCM	Meteorologic and hydrologic data, hourly storm or storm sequence Land use and soil parameters BMP information	Daily runoff and pollutant loads BMP removal efficiencies
Auto QI	Hourly/daily rainfall Watershed and land use data BMP removal rates	Continuous or storm event simulation of runoff and selected pollutants
AGNPS	Watershed, land use, management and soil data Rainfall data, topography BMP removal data	Storm runoff volume and peak flow Sediment, nutrient, and COD concentrations
SLAMM	Hourly rainfall data Pollution source characteristics areas soil type, imperviousness, and traffic Structure characteristics	Pollutant load by source area BMP evaluation and cost estimates

Table 11 Input and Output Data - Detailed Models

Models	Main Input Data	Output Information
STORM	Hourly rainfall data Buildup and wash-off parameters Runoff coefficient and soil type	Event-based runoff and pollutant loads Storage and treatment utilization and number of overflows Hourly hydrographs and pollutographs
ANSWERS	Hourly rainfall data Watershed, land use, and soil data BMP design data	Predicts storm runoff (volume and peak flow) Sediment detachment and transport Analysis of relative effectiveness of agricultural BMPs
DR3M QUAL	Meteorologic and hydrologic data Watershed characteristics related to runoff Channel dimensions and kinematic wave parameters Characteristics of storage basins Buildup and wash-off coefficients	Continuous series of runoff and pollutant yield at any location in the drainage system Summaries for storm events Hydrographs and pollutographs
SWRRBW Q/SWAT	Meteorologic and hydrologic data Watershed and receiving waterbody parameters Land use and soil data Pond and reservoir data	Continuous water and sediment yield Peak discharge Water quality concentrations and loads
SWMM	Meteorologic and hydrologic data Land use distribution and characteristics Accumulation and wash off parameters Decay coefficients	Continuous and event-based runoff and pollutant loads Transport through streams and reservoirs Analysis of control strategies

Table 12 Input Data Needs for Watershed Models

1 System Parameters
   - Watershed size
   - Subdivision of the watershed into homogenous subareas
   - Imperviousness of each subarea
   - Slopes
   - Fraction of impervious areas directly connected to a channel
   - Maximum surface storage (depression plus interception storage)
   - Soil characteristics including texture, permeability, erodibility, and composition
   - Crop and vegetative cover
   - Curb density or street gutter length
   - Sewer system or natural drainage characteristics

2 State Variables
   - Ambient temperature
   - Reaction rate coefficients
   - Adsorption/desorption coefficients
   - Growth stage of crops
   - Daily accumulation rates of litter
   - Traffic density and speed
   - Potency factors for pollutants (polutant strength on sediment)
   - Solar radiation (for some models)

3 Input Variables
   - Precipitation
   - Atmospheric fallout
   - Evaporation rates

Source After Novotny and Chester, 1981

Table 13 Range of Application of Watershed Models-Simple Methods

Simple Methods	Watershed Analysis			Control Analysis		Receiving Water Quality
	Screening	Intermediate	Detailed	Planning	Design	
EPA Screening	●	-	-	-	-	○
The Simple Method	●	-	-	○	-	-
Regression	●	-	-	-	-	-
SLOSS/ PHOSPH	○	-	-	-	-	-
Watershed	●	-	-	○	-	-
FWHA	●	-	-	○	-	○
WMM	●	○	-	◒	-	◒

● High ◒ Medium ○ Low - Not Available

Table 14 Range of Application of Watershed Models-Simple Methods

Mid-Range Methods	Watershed Analysis			Control Analysis		Receiving Water Quality
	Screening	Intermediate	Detailed	Planning	Design	
SITEMAP	●	○	○	◒	-	○
GWLF	●	◒	○	-	-	-
P8-UCM	●	◒	◒	○	●	-
Auto-QI	●	●	○	◒	○	○
AGNPS	●	●	○	●	○	○
SLAMM	●	◒	◒	●	◒	○

● High ◒ Medium ○ Low - Not Incorporated

Table 15　Range of Application of Watershed Models-Detailed Methods

Detailed Methods	Watershed Analysis			Control Analysis		Receiving Water Quality
	Screening	Intermediate	Detailed	Planning	Design	
STORM	●	●	○	●	○	○
ANSWERS	●	●	◒	●	○	○
DR3M-QVAL	◒	●	●	●	◒	◒
SWRRBQ/ SWAT	◒	●	●	●	◒	◒
SWMM	◒	●	●	●	◒	-
HSPF	◒	●	●	●	◒	●

● High　◒ Medium　○ Low　- Not Incorporated

(五)總量管制承受水體模式應用及選擇

在此種模式去模擬承受水體反應考慮事項為1 水體種類2 水體流率是穩態或動態3 需被模擬之各種水動力水質、毒性和沉澱步驟4 被參數修正、校正及建立可運用之數據。水動力模式，穩態水質模式及動態水質模式主要之物理、化學、被模擬參數及水文資料應用如表16、17及18。水動力模式、穩態水質模式及動態水質模式主要輸入及輸出數據應用如表19、20及21。水動力模式、穩態水質模式及動態水質規劃應用、設計分析列於表22、23及24。

(六)總量管制生物評估模式應用及選擇

如同流域負荷模式及承受水體模式選擇及應用相似，生物評估模式需考慮以下幾個因素

1 目標　包括目前狀況評估、河川復原優先排列計畫　土地利

用改變未來情形之預測。

2 目的　包括決定及預測棲息地種類、棲息地的品質和數量，居住種類完整性。

3 完成目標詳細程度　包括簡單、中度及複雜三種。

4 數據可利用性　包括參考情況。

5 擁有其他生物評估、承受水體模式及負荷之可應用性。

6 專家所需之程度，許多技巧需要專業生物學家去收集及分析數據。

7 考慮成本。

以下之表列數據能幫助評估及選擇適當技巧對於集水區之評估及總量管制之發展。表25及26提供一技術成分詳實描述包括生物及棲息地之評估及方法論。表27及28呈現一簡短之輸入及輸出方法對每一種步及模式而言。表29及30呈現生物評估技巧及模式之潛在應用範圍包括陸地上、海域及濕地之生物棲息地評估，和深海底生物群聚，魚類群聚及生物累積和群聚模式之評估。

Table 16 A Descriptive List of Model Components-Hydrodynamic Models

Model	Dimension	Horizontal Coordinate System	Vertical Coordinate System	Vertical Mixing	Solution Technique
Externally Couple					
RIVMOD H	1-D	N/A	N/A	N/A	Implicit
dynhyds	1-d	Link Node	N/A	N/A	Explicit Runge-Kutta
EFDC	1-D, 2-D (x/y, x/z), 3-D	Cartesian, orthogonal boundary fitted, laterally averaged	Staircase Cartesian, sigma transformation to local bathymetry	Turbulence closure	Implicit
CH3D WES	1-D, 2-D (x/y, x/z), 3-D	Cartesian, orthogonal boundary fitted, laterally averaged	Staircase Cartesian	Turbulence closure	Implicit
Internally Coupled					
CE-QUAL-RIV1	1-D	N/A	N/A	N/A	Implicit (RIV1H)
CE-QUAL W2	1-D 2-D (x/z)	Cartesian laterally averaged	Staircase Cartesian	Wind shear	Implicit
HSPF	1-D	N/A	N/A	N/A	Implicit

Table 17 A Descriptive List of Model Components-Steady-State Water Quality Models

Model	Waterbody Type	Parameters Simulated	Processes Simulated	
			Physical	Chemical/Biological
EPA Screening Methods	River, lake/ reservoir, estuary, coastal	Waterbody nitrogen, phosphorus, chlorophyll or chemical concentrations	Dilution, advention, dispersion	First-order decay empirical relationships between nutrient loading and eutrophication indices
EUTROMOD	Lake/reservoir		Dilution	Empirical relationships between nutrient loading and eutrophication indices
PHOSMOD	Lake/reservoir	DO, phosphorus	Dilution	Empirical relationships between nutrient loading and eutrophication indices
BATHTUB	Lake/reservoir	DO, nitrogen, phosphorus, chlorophyll	Dilution	Empirical relationships between nutrient loading and eutrophication indices
QUALZE	Rivers, (well-mixed/ shallow lakes or estuaries)	DO, CBOD, temperature, organic N ammonia, nitrite nitrate, organic P, dissolved phosphorous, phytoplankton, fecal coliform arbitrary nonconservative substances, three conservative substances	Dilution, advection dispersion, heat balance	First-order decay, DO-BOD cycle nutrient-algal cycle
EXAMSII	Rivers	Conservative and nonconservative substances	Dilution advection, dispersion	First-order decay, process kinetics, daughter products, exposure assessment
TOXMOD	Lake/reservoir	Conservative and nonconservative substances	Dilution, advection, dispersion	First-order decay, sediment burial and release
SYMPTOX4	River/reservoir	Conservative and nonconservative substances	Dilution, advection, dispersion	First-order decay, sediment exchange
TPM	Estuaries	DO, CBOD, NBOD, temperature, ammonium, nitrate, nitrite, organic nitrogen, total phosphate organic phosphorus, salinity, inorganic suspended solids, dissolved labile, and refractory particulate organic carbon, dissolved silica, particulate biogenic silica, fecal coliform, total active metal	Dilution, advection, dispersion, heat balance, particle fate	First-order decay, DO-BOD cycle, nutrient-algal cycle, carbon cycle, silica cycle, benthic algae, sediment digenesis
DECAL	Coastal	Sediment, conservative and nonconservative substances	Dilution, advection, dispersion, particle fate	First-order decay,

Table 18 A Descriptive List of Model Components-Dynamic Water Quality Models

Model	Waterbody Type	Parameters Simulated	Processes Simulated	
			Physical	Chemical/Biological
DYNTOX	River	Conservative and nonconservative substances	Dilution, advention	First-order decay
WASPS	Estuary, river (well mixed/ shallow lake)	DO, CBOD, NBOD, ammonium, nitrate, nitrite, organic nitrogen, total phosphate, organic phosphorus, inorganic suspended solids, fecal coliform, conservative and nonconservative substances	Dilution, advection, dispersion, reaeration	First-order decary process kinetics, daughter products, hydrolysis, oxidation volatilization, photolysis, equilibrium adsorption Settling, DO-CBOD, nutrient algal cycle
CE QUAL-RIV1	Rivers	DO, CBOD, temperature, ammonia, nitrate, algae, coliform, phosphate, organic nitrogen	Dilution, advection, dispersion, heat balance	First order decay, DO-CBOD, nutrient algal cycle
CE-QUAL-W2	Lakes	DO, CBOD, NBOD, temperature, ammonium, nitrate, nitrite, organic nitrogen, total phosphate, organic phosphorus, salinity, inorganic suspended solids, dissolved labile, and refractory particulate organic carbon, dissolved silica, particulate biogenic silica, fecal coliform, total active metal	Dilution, advection, dispersion, heat balance	First-order decay, DO-CBOD, nutrient-algal cycle, carbon cycle
CE-QUAL-ICM	Estuaries, rivers, lakes, coastal	DO, CBOD, NBOD, temperature, ammonium, nitrate nitrite organic nitrogen total phosphate, organic phosphorus, salinity, inorganic suspended solids, dissolved labile, and refractory particulate organic carbon, dissolved silica, particulate biogenic silica, fecal coliform, total active metal	Dilution, advection, dispersion heat balance, particle fate, sediment digenesis	First-order decay, DO-BOD, nutrient-algal cycle carbon cycle, silica cycle, zoo-plankton, sediment digenesis
HSPF	River, (well-mixed/shallow lakes)	DO, BOD nutrients, pesticide sediment, organic chemicals, and temperature	Dilution advection, heat balance, particle fate, cohesive/ noncohesive sediment transport	First-order decay process kinetics, daughter products hydrolysis, oxidation volatilization, photolysis, benthic demand respiration, nutrient-algal cycle

Table 19 Input and Output Data - Hydrodynamic Models

Model	Main Input Data	Output Information
Externally Coupled		
RIVMOD-H	River geometry and boundary conditions, inflows, withdrawals, meteorologic data	Water surface elevations velocities, and temperatures
DYNHYD5	Waterbody geometry and boundary conditions, inflows withdrawals, meteorologic data	Water surface elevations, velocities
EFDC	River geometry, bathymetry geometric data, grid system, and boundary conditions inflows, withdrawals, meteorologic data	Water surface elevations, velocities magnitude and orientation temperature salinity, and conservative tracer
CH3D-WES	River geometry, bathymetry, geometric data, grid system and boundary conditions, inflows, withdrawals, meteorologic data	Water surface elevations, velocity magnitude and orientation temperature
Internally Coupled		
CE-QUAL-RIV1	River geometry and boundary conditions, inflows, withdrawals, meteorologic data	Water surface elevations velocities, and temperatures
CE-QUAL-W2	Waterbody geometry, bathymetry, and boundary conditions, inflows, withdrawals, meteorologic data	Water surface elevations velocities longitudinal and vertical, and temperature
HSPF	River geometry and boundary conditions, inflows, withdrawals, meteorologic data	Water surface elevations velocities, and temperatures

Table 20 Input and Output Data - Steady-State Water Quality Model

Model	Main Input Data	Output Information
EPA Screening Methods	Climate, waterbody morphometry, external loading	Waterbody nitrogen, phosphorus, chlorophylla, or chemical concentrations
EUTROMOD	Climate, lake morphometry, watershed characteristics (land use)	Lake DO, nitrogen, phosphorus, and chlorophylla concentrations
PHOSMOD	Climate, lake morphometry, external loading, benthic flux	Lake DO, phosphorus, and chlorophylla concentrations
BATHTUB	Climate lake morphometry external loadings	Lake DO, nitrogen phosphorus, and chlorophylla concentrations
QUAL2E	Climate, river geometry, stream network, flow, boundary conditions, 26 physical, chemical and biological properties for each reach, inflows/ withdrawals	DO, CBOD, nitrogen, phosphorus conservative and nonconservative constituent concentrations
EXAMSII	Stream geometry, flow, chemical loadings, total pollutant and suspended solids concentrations physical/ chemical coefficients	Chemical exposure, fate and persistence
TOXMOD	Lake morphometry, initial conditions external loadings, benthic flux	Conservative and nonconservative substance concentrations
SYMPTOX4	Stream geometry, flow, total pollutant and suspended solids concentrations, physical/ chemical coefficients and rates	Conservative and nonconservative substance concentrations in total, dissolved and particulate forms, in the water column and bed sediments Suspended solids concentration in water column
TPM	Climate geometric data boundary conditions, up to 140 parameters for full simulation of water quality kinetics	DO CBOD NBOD temperature ammonium, nitrate, nitrite, organic nitrogen total phosphate organic phosphorus, salinity, inorganic suspended solids, dissolved labile, and refractory particulate organic carbon, dissolved silica particulate biogenic silica fecal coliform, total active metal
DECAL	Coastal geometry tidal oscillations loadings initial and boundary conditions	Contour plots of suspended particle concentrations in lower water layers Daily averaged deposition rates of organic material

Table 21 Input and Output Data - Dynamic Water Quality Model

Model	Main Input Data	Output Information
DYNTOX	River geometry, flow (continuous records or statistical summaries), external loadings boundary conditions	Conservative and nonconservative substance concentrations, plots of return period for water quality violations below each discharge
WASP5	Waterbody geometry climate, waterbody segmentation, flow (or input from hydrodynamic model), boundary conditions, initial conditions, benthic flux, external loadings, spatially variable and time-variable functions, rate constants	DO, CBOD, NBOD, ammonium, nitrate, nitrite, organic nitrogen, total phosphate, organic phosphorus, inorganic suspended solids, fecal coliform, conservative and nonconservative substance concentrations for each segment and user-defined time interval
CE-QUAL-RIV1	River geometry, climate, river segmentation, upstream boundary conditions, initial conditions, external loadings, benthic flux, spatially variable and time-variable functions, rate constants	DO, CBOD, temperature, ammonia nitrate, algae, coliform, phosphate, organic nitrogen concentrations for each segment and user-defined time interval
CE-QUAL-W2	Lake geometry, climate waterbody segmentation, boundary conditions, initial conditions external loadings or withdrawals, benthic flux, spatially variable and time-variable functions, rate constants	DO, CBOD, NBOD temperature, ammonium, nitrate, nitrite, organic nitrogen, total phosphate organic phosphorus, salinity, inorganic suspended solids, dissolved, labile, and refractory particulate organic carbon, dissolved silica particulate biogenic silica, fecal coliform, total active metal concentrations for each segment and user-defined time interval
CE-QUAL-ICM	Waterbody geometry, climate, grid, flow (or input from hydrodynamic model), boundary conditions, initial conditions, external loadings, spatially variable and time variable functions, rate constants	DO, CBOD, NBOD, temperature, ammonium, nitrate, nitrite, organic nitrogen, total phosphate, organic phosphorus, salinity inorganic suspended solids, dissolved, labile, and refractory particulate organic carbon, dissolved silica. particulate biogenic silica, fecal coliform total active metal concentrations for each segment and user-defined time interval
HSPF	River, well-mixed/shallow lakes	DO, CBOD, nutrients, pesticide, sediment and organic chemical concentrations for each segment and user-defined time interval

Table 22 Range of Application--Hydrodynamic Models

Model	Hydrodynamic Analysis			Water Supply-Control Analysis Operations/ anagement	
	Screening	Intermediate	Detailed	Planning	Design
Externally Coupled					
RIVMOD-H	●	◒	○	●	◒
DYNHYD5	●	●	○	○	-
EFDC	○	◒	●	●	◒
CH3D-WES	○	◒	●	●	◒
Internally Couple					
CE-QUAL-RIV1	●	◒	○	◒	○
CE-QUAL-W2	○	●	●	●	●
HSPF	◒	●	◒	◒	◒

● High ◒ Medium ○ Low - Not Incorporated

Table 23 Range of Application--Steady-State Water Quality Models

Model	Screening	Intermediate	Detailed	Management Planning and Analysis
EPA Screening Methods	●	○	-	○
EUTROMOD	●	◒	-	◒
PHOSMOD	●	◒	-	◒
BATHTUB	●	◒	-	◒
QUALZE	●	●	◒	●
EXAMSII	●	●	-	◒
TOXMOD	●	◒	-	◒
SMPTOX3	●	◒	◒	●
TPM	●	●	◒	●
DECAL	●	●	◒	●

● High ◒ Medium ○ Low - Not Incorporated

Table 24 Range of Application--Dynamic Water Quality Models

Model	Water Quality Analysis			Management Planning and Analysis
	Screening	Int	Detailed	
DYNTOX	●	○		○
WASP5	○	●	○	●
CE-QUAL-RIV1	●	●	●	●
CE-QUAL-W2	○	●	●	●
CE-QUAL-ICM		◒	●	●
HSPF	○	◒	●	●

● High ◒ Medium ○ Low - Not Incorporated

Table 25 A Descriptive List of Model/Technique Components - Habitat Assessment Techniques

Technique/ Model	Habitat Type assessed	Habitat Parameter	Habitat Level Assessed	Methodology
HEP/HIS	Terrestrial/ quatic	Quantity and quality	Single or multiple species	Modeling of habitat quantity and quality using key parameters collected from field can simulate effects of future
HES	Terrestrial/ aquatic	Quantity and quality	Community	Modeling of habitat quantity and quality using abiotic and biotic field collected data, can simulate effects of future
WET II	Wetland	Quality	Single or multiple species	Collection and analysis of physical, chemical, and biological predictors to assess wetland functions
HGM	Wetland	Quality	Community	Data collection and classification, development and comparison to reference conditions
Visual-based Habitat Assessment	Aquatic	Quality	Community	Multimetric collection and analysis, comparison to reference conditions
OHEI	Aquatic	Quality	Community	Multimetric collection and analysis comparison to reference conditions
Rosgen's Stream Classificatio	Aquatic	Quantity and quality	N/A	Collection and analysis of morphological stream data, classification to predict stream behavior
IFIM (PABSIM/ TSLIB)	Aquatic	Quantity and quality	Single or multiple species	Modeling of aquatic habitat quantity and quality using key parameters collected from field, can simulate effects of future development/conditions
SNTEMP/ SSTEMP	Aquatic	Quality	N/A	Modeling of stream temperature using stream geometric, hydrologic, and meteorologic data

Table 26 A Descriptive List of Model/Technique Components - Species/ Biological Community Assessment Techniques

Technique/ Model	Biota Assessed	Data Source	Methodology
RBP I	Benthic macroinvertebrates	Field	Visual only
RBP II	Benthic macroinvertebrates	Field	Analysis of eight metrics in the field, comparison to reference conditions
RBP III	Benthic macroinvertebrates	Field	Analysis of eight metrics in the field and laboratory, comparison to reference conditions
RBP IV	Fish	Questionnaire	Analysis of questionnaire data
RBP V (IBI)	Fish	Field	Analysis of 12 metrics in the field, comparison to reference conditions
ICI	Benthic macroinvertebrates	Field	Analysis of 10 metrics in the field, comparison to reference conditions
IWB	Fish	Field	Analysis of species abundance and diversity in the field, comparison to reference conditions
PVA	Any	Field/literature	Modeling of wildlife population stability using data describing birth, death, and growth rates
FGETS	Any	Field/literature	Modeling of fish bioaccumulation of chemicals based on biological attributes and physicochemical properties

Table 27 Input and Output - Habitat Assessment Techniques

Technique/ Model	Output Information	Main Input Data
HEP/HIS	A quantitative assessment of the quality and quantity of available habitat for selected wildlife species in terms of proposed or anticipated land use changes, and the cost-effectiveness of different management alternatives to achieve desired HUs for a selected species	Data to be collected include delineation of cover types (e g , deciduous forest, coniferous forest, grassland, residential woodland) within the project area, size (acreage) of existing habitat for each evaluation species, selection of evaluation species, Habitat Suitability Index (HIS) reflecting current habitat conditions for each evaluation species, future habitat conditions for each evaluation species HIS data collection includes (1) species-specific habitat use information such as general information (e g geographic distribution), age, growth, and food requirements, water quality, depth and flow, species-specific habitat requirements reproductive information, (2) species-specific life history information for each life stage (spawning/ embryo, fry, juvenile, and adult), (3) suitability indices for each habitat variable
HES	A quantitative assessment of the quality and quantity of available habitat for entire wildlife communities in terms of proposed or anticipated land use changes	Baseline data on habitat types and land uses in the project area Size (acreage) of each habitat type and land use for existing and future conditions Measurements of key variables (e g , percent understory, number of large trees, number of mast trees, species associations, number of snags) identified for each habitat and land use type for existing conditions Projected measurements of same key variables for future conditions
WET II	A "broad-brush," quantitative assessment of potential project impacts on several wetland habitat functions	Baseline data (e g , water source, hydrodynamics, surface roughness, vegetation cover, soil type) characterizing the following wetland functions and values groundwater discharge, groundwater recharge sediment stabilization, flooa flow alteration, sediment retention, toxicant retention, nutrient transformation, production export, wildlife diversity, aquatic diversity, recreation, uniqueness/heritage
HGM	A quantitative assessment of the functioning of wetlands that uses the concepts of hydrogeomorphic classification, functional capacity, reference domain, and reference wet/ands	Baseline data to develop a reference set of wetlands representing the range of conditions that exist in a wetland ecosystem and its landscape in a reference domain Baseline data on the condition of assessment wetland variables (e g surface and subsurface water storage, nutrient cycling retention of particulates, organic matter export, spatial structure of habitat, distribution and abundance of invertebrates and vertebrates, plant community characteristics etc) measured directly or indirectly using indicators to develop a relationship between variable conditions in the assessment wetland and functional capacity of the reference set
Visual based Habitat Assessment	A quantitative assessment, based on qualitative information, of aquatic habitat quality in wadable streams and rivers	Data to be collected include instream cover (fish) (riffle/run only), bottom substrate/available cover (glide/pool only), epifaunal substrate (riffle/run only), pool substrate chactenzation (glide/pool only), embeddedness (riffle/run only), pool variability (glide/pool only), channel alteration sediment deposition, frequency of riffles (riffle/run only), channel sinuosity (glide/pool only), channel flow status, bank vegetative protection, bank stability, riparian vegetative zone width

Table 27-1 Input and Output - Habitat Assessment Techniques(continued)

Technique/ Model	Output Information	Main Input Data
QHEI	A quantitative assessment based on qualitative information Developed to help distinguish the influence of habitat effects on fish communities in midwestern streams	Data to be collected include substrate (type, origin, and quality), instream cover (type and amount), channel morphology (sinuosity, development, channelization, stability, modifications/other), riparian zone and bank erosion (riparian width, floodplain quality and bank erosion), glide/pool and riffle/run quality (max depth, morphology, current velocity, riffle/run depth, riffle/run substrate, and riffle/run embeddendness) gradient, drainage area, percent pool, percent glide, percent riffle, percent run
Rosgen's Stream Classification	A quantified classification system that can be used to predict stream behavior and to apply interpretive information Interpretations can be used to evaluate a stream's sensitivity to disturbance, recovery potential, sediment supply, vegetation controlling influence, and streambank erosion potential	Data to be collected depend on the level of classification Level 1 landform, lithology, soils, climate, depositional history, basin relief, valley morphology, river, profile morphology general river pattern Level 2 channel pattern, sinuosity (usually expressed as Schumm's ratio), gradient or slope, entrenchment or entrenchment ration (width of floodplain the bankfull width of channel surface), channel bed material, width/depth ratio Level 3 riparian vegetation, depositional patterns, meander patterns, confinement features, fish habitat indices, flow regime, river size category, debris occurrence, channel stability index, bank erodibility
IFIM (PHABSIM /TSLIB)	A quantitative assessment (usually in graphical form) of the changes in a given species' habitat with changes I hydrologic regime	Detailed data collection is required for both physical (e g depth velocity, stream channel characteristics, riparian cover) and biological (e g , life history and habitat preference information for the species of concern) characteristics of the stream
SNTEMP/SSTEMP	Minimum, mean, and maximum daily water temperature for a stream segment	20 input parameters are required that describe the stream geometry (e g , segment length, elevation, roughness, shading), hydrology (e g , segment inflow and outflow dam locations), and meteorology (e g , air temperature, relative humidity, solar radiation)

Table 28 Input and Output - Species/Biological Community Assessment Techniques

Technique/Model		Output Information	Main Input Data
Screening level approaches	RBP I	Based on a macroinvertebrate community assessment, RBP I determines whether an impairment exists in a stream (or whether further investigation is needed) and gives a generic indication of impairment cause (e g , habitat, organic enrichment, toxicity)	Characterize and rate substrate/instream cover, channel morphology, and riparian/bank structure, measure conventional water quality parameters, examine physical characteristics, determine relative abundance of benthic macroinvertebrates
	RBP IV	Based on a fish community assessment, RBP IV determines whether an impairment exists in a stream (or whether further investigation is needed) and givers a generic indication of impairment cause	Characterize and rate substrate/instream cover, channel morphology, and riparian/bank structure, measure conventional water quality parameters, examine physical characteristics, questionnaire survey regarding fish communities survey ecoregional reference reaches and randomly selected streams
Multimetric approaches	RBP II	Based on benthic macroinvertebrate collection and analysis, RBP II characterizes the severity of an impairment into one of three categories, gives a generic indication of its cause, and ranks and prioritizes streams of further assessment	Characterize and rate substrate/instream cover, channel morphology, and riparian/bank structure, measure conventional water quality parameters, examine physical characteristics, examine riffle/run community and sample coarse particulate organic matter, 100-organism subsample indentified in field to family or order level, functional feeding group analysis of riffle/run and coarse particulate organic matter in the field Data describing reference conditions are also necessary
	RBP III	Based on benthic macroinvertebrate collection and analysis, RBP III characterizes the severity of an impairment into one of four categories, gives a generic indication of its cause establishes a basis for trend monitoring, and prioritizes streams for further assessment	Characterize and rate substrate/instream cover, channel morphology, and riparian/bank structure, measure conventional water quality parameters, examine physical characteristics, examine riffle/run community and sample coarse particulate organic matter, collect riffle/run benthos, collect coarse particulate organic matter sample, determine shredder abundance, perform riffle/run analysis in laboratory, identify 100 organism subsample to species level and perform functional feeding group analysis Data describing reference conditions are also necessary
	ICI	ICI provides a quantitative measure of overall macroinvertebrate community condition	Data necessary for development of the ICD include total number of taxa, number of mayfly taxa, number of caddisfly taxa, number of dipteran taxa, percent mayfly composition, percent caddisfly composition percent tribe tanytarsini midge composition percent other diptera and noninset composition, percent tolerant organisms, and number of qualitative EPT taxa Data for reference conditions are also necessary

Table 28-1 Input and Output - Species/Biological Community Assessment Techniques(continued)

Technique/Model		Output Information	Main Input Data
Multimetric approaches (continued)	RBP V (IBI)	Based on fish collection and analysis, RBP V computes a quantitative index that incorporates individual, population, community, zoogeographic, and ecosystem level information to evaluate biological integrity as one of five classes, it also gives a generic indication of impairment cause establishes a basis for trend monitoring, and ranks and prioritizes streams for further assessment	Data to be collected include substrate/instream cover, channel morphology, and riparian/bank structure, conventiaonal water quality parameters, physical characteristics, major habitats and cover types, total number of native fish species, number and identity of darter species, number and identity of sunfish species, number and identity of sucker species, number and identity of intolerant species, proportion of individuals as tolerant species, proportion of individuals as omnivores, proportion of individuals as insectivorous cyprinids, proportion of individuals as piscivores (top carnivores), number of individuals in sample, proportion of individuals as hybrids, proportion of individuals with disease tumors fin damage, and skeletal anomalies Data describing reference conditions are also necessary
	IWB	The IWB provides a quantitative measure of the quality of a fish assemblage	Data to be collected include number of individuals/kilometer, biomass of individuals/kilometer, Shannon-Weaver diversity index (number of individuals in sample and number of individuals of species in the sample) Data describing reference conditions are also necessary
Population Viability Analysis (PVA)		PVAs supply a quantified analysis of the stability of a specified population following a change in environment, population structure, or behavior	Data required include the age structure of the population being studied, and the survival and fecundity of each age
FGETS		FG ETS predicts the temporal dynamics of a fish's whole-body concentration of nonionic, nonmetabolized, organic chemicals that are bioaccumulated from water and food	Data required include morphological, physiological, and trophic parameters that describe the gill morphometry, feeding and metabolic demands, and body composition for the species in questions, and relevant physicochemical parameters that describe partitioning to the fish's lipid and structural organic fractions for a specific chemical

Table 29 Range of Application - Habitat Assessment Techniques and Models

Technique/Model	Habitat Assessment		
	Terrestrial	Aquatic	Wetland
HEP/HIS	●	◒	-
HES	●	●	-
WET II	-	-	●
HGM	-	-	●
Visual-based Habitat Assessment	-	○	-
QHEI	-	○	-
Rosgen's Stream Classification	-	◒	-
IFIM (PHABSIM/TSLIB)	-	●	-
SNTEMP/SSTEMP	-	◒	-

Level of complexity addressed ● High ◒ Medium ○ Low - Not Applicable

Table 30 Range of Application - Species/Biologic al Community Assessment Techniques and Models

Technique/Model	Assessment Type		
	Benthic community	Fish community	Single-species (Bioaccumulation and population modeling)
RBP I	○	-	-
RBP II	◒	-	-
RBP II	●	-	-
RBP IV	-	○	-
RBP V (IBI)	-	●	-
ICI	◒	-	-
IWB	-	◒	-
PVB	-	-	●
FGETS	-	-	●

Level of complexity addressed ● High ◒ Medium ○ Low - Not Applicable

八、總量管制模式之率定

(一)總量管制模式之涵容能力分析建立

河川模式分析目前仍是以BOD-DO模擬為主，故河川的涵容能力定義為在下影響河川正常水體之用途條件下，河川每日所能排入之BOD量。涵容能力之計算基準因每條河川之用途不盡相同，應根據法令規定之水體標準來計算各河川容許之污染量，選擇適當之設計流量及設計溫量。

計算河川涵容能力之步驟如下所列

1 河川基本資料之收集(水質調查及水理調查)。
2 選取設計流量。
3 收集污染原資料（包括原始污染負荷量及流達率）。
4 選取已通過檢定、驗證之水質模式。
5 選定水質模擬點。
6 估算涵容能力。

(二)總量管制之模式建立

利用水質數學模式進行水污染研究第一步為模式之建立，也即依水體及污染物之特性，將控制方程式寫出，選擇一個適當的解法，寫成電腦程式，並進行程式之試跑、偵錯。模式種類之選擇應該依照所需精確度、可研究之時間、可用之錢數、電腦種類、資料之多寡等各種因素而決定。也可利用別人已建立發展之模式，以節省時間、人力。複雜的模式並

不是最好的模式，若野外數據充足，利用程式的人（Modeler）有能力及時間，則複雜的模式可以產生較詳細、精確的結果，幫助吾人進行更好的工程規劃、設計。如前所述，有時簡單的模式，已足夠我們的精度需求，如果野外數據不多，水體複雜性低，時間、金錢不足時，可以選擇比較簡單的模式。

(三)總量管制模式建立之檢定（Calibration）

模式建立建展完成後，第二階段為檢定模式中之係數、參數，也即利用一組野外實測數據為依據，改變模式中之參數、係數，一直至模式之結果與實測數據吻合或接近為止，以決定模式中最適當之係數、參數。當然，工作中包括輸入一個水體之水文、幾何條件與已知之邊界起始條件。

複雜的模式中，係數種類多（可能有數十個），且互相牽制，因此為一繁雜的工作。也可用優選法來推求最佳參數值，此即為反向推求問題。

(四)總量管制模式建立之驗證（Verification）

模式經過檢定後，為了增加對模式準確度之信心，需有驗證工作。模式之驗證需要另外一組野外實測資料（如河川之BOD、DO），將另一組獨立（即不同於檢定時之情況）的輸入資料、邊界條件等輸入模式，將所得之結果（即BOD、DO之濃度分佈）與實測資料比較，若吻合情況良好，則可以設

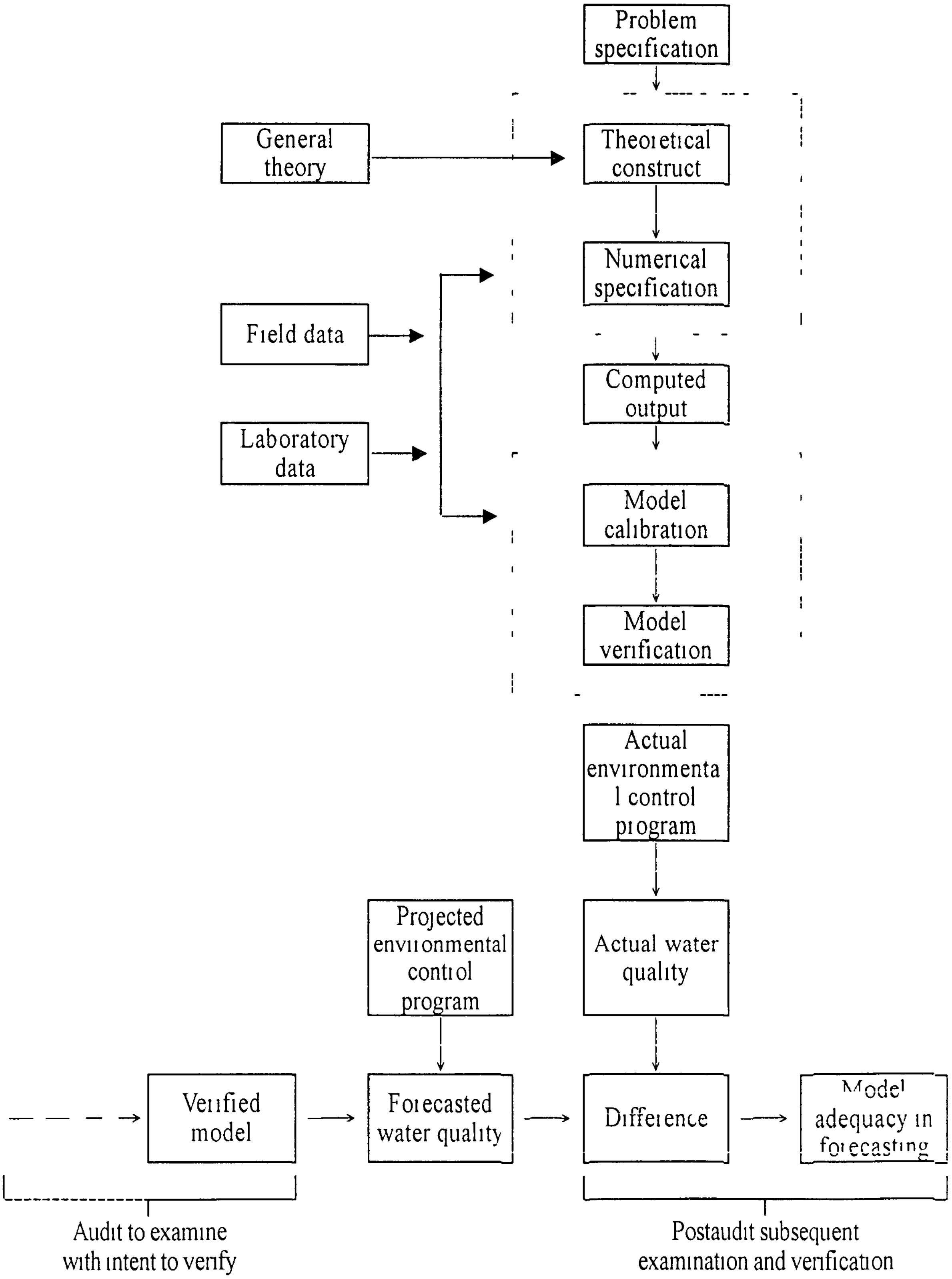
模式之準確性已被驗證，若結果相差太多，則模式還是有瑕疵，需再研判其原因。

(五)總量管制模式建立之敏感度分析（Sensitivity Analysis）

為了瞭解模式中所用之參數、係數對模擬結果之重要性，可再進一步進行敏度分析。其過程為改變係數、參數之值，決定模擬結果之改變幅度大小為何？若係數之微小差異引致模擬結果大變動，則可知道此係數對模式很重要，給我們指引，可能要進一步瞭解此係數之正確值（譬如實地量取或進行室內、室外實驗），以增加模式結果之正確性。反之，則表示此係數值對模式結果之影響較不重要。敏感度分析也可幫助我們進行水質規劃、分析。

(六)總量管制模式建立之應用

模式經過前面五個階段，便可被利用來作各種情況之水質模擬、預測、分析、研究，甚至被利用於優選模式中之物理限制式（Physical constraints）模式架構組織如圖3。根據這些模擬結果，可用來幫助吾人設計合乎經濟原則之污水處理廠、管制廢水排放、總量分配等之總量管制，這也是模式的最後目的與主要功用。



Figue 3 Principal components of modeling framework (a) Steps up through verification (b) Postaudit of models

九、點源與非點源總量管制模式應用

(一)點源對總量管制模式應用

傳統之總量管制是指管制各點源每日排放出來之污染量不得超過容許排放量。而各污染源容許排放量大部分是根據下面方法決定的

1 使用水質模式求水體的涵容能力（assimilative capacity）

2 決定水體涵容能力的保留容量，一般保留15%至30%

3 水體的涵容能力減去保留容量得容許排入總量

4 考慮各污染源的大小、廢水處理的難易度、處理成本、公平性等因素，將容許排入總量分配給各污染源，即為各污染源的容許排放量，環保單位再依此容許排放量管制各污染源。此即為總量管制。

由上面步驟可知，水質模式是應用在求水體的涵容能力上。水質模式可分為確定模式(determinate models)和機率模式(stochastic models)兩大類，但以前者較常用。確定模式多是由質量平衡(mass balance)原理導出，依水體水質和水理變動情形，模式可分為定常模式與動態模式，若依維度分可分為零維、一維、二維和三維。最早且最有名之水質模式為1925年美國人Streeter-Phelps之河水的DO-BOD模式。通常很少用三維模式，較複雜之二維動態模式為

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(UxC) - \frac{\partial}{\partial z}(UzC) + \frac{\partial}{\partial x}\left[Ex\frac{\partial C}{\partial x}\right] + \frac{\partial}{\partial z}\left[Ez\frac{\partial C}{\partial z}\right] \pm S(x\ z\ t) \qquad (1)$$

式中，C=水質濃度$[M/L^3]$

t=時間[T]

U_1=流速[L/T]

E_1=擴散係數$[L^2/T]$

S=生成或消失項$[M/L^3/T]$

(1)式中右邊前二項代表傳流項，為水流對物質產生的傳遞。三、四項為擴散項，代表物質在水中受擴散，紊流等所產生的傳遞。最後一項則代表該物質本身的生化反應現象，此項隨模擬物質的不同而異。

二維模式常用於水庫和感潮河川，非感潮河川只用一維模式即可。一維模式將(1)式中有關z變數去掉即可(即對z取平均)。由於動態模式多為二次微分方程式加上動量與連續而水力方程式，不易求得解析解，故用數值解法。由於數值解法方法很多，加上(1)式最後一項所考慮的生化反應的不同，因此有許多之水質模式產生。較常用的動態水質模式有QUAL-IIE、WASP、CE-QUAL-W2，或是專門用在感潮河川之ESTURY等。美國EPA最新發展出來的BASIN套裝模式，就是結合GIS與HSPF、QUAL-IIE而成，HSPF用來估計集水區產生點源與非點源之污染量，再用QUAL-IIE模擬水體水質和計算TMDL(Total Maximum Daily Loads)，進一步以總量管制各污染源。

(二)非點源對總量管制模式應用

主要非點源模式有SWMM、STORM、AGNPS、ANSWERS

、HSPF VAST及VANTU等數種模式，其中模擬單場降雨者除STORM外其它模式皆可模擬，模擬連續降雨者為SWMM、STORM及HSPF，模擬SS除AGNPS外皆可，有機物BOD及COD除AGNPS和ANSWERS較差外，其餘皆可模擬，氨氮該等模式皆可模擬，總磷除ANSWERS和VANTU外其餘模式皆可模擬，DO僅SWMM、HSPF、VAST及VANTU等模式可模擬，模擬能力SWMM、HSPF、VAST為較優者，STORM、AGNPS、ANSWERS尚可，數據及人力需求SWMM、AGNPS、ANSWERS、HSPF為較高者，VAST及VANTU為中等，而STORM所需較少，另模式複雜度以SWMM、HSPF較複雜，而STORM、AGNPS、ANSWERS、VAST和VANTU為中等。詳細主要非點源總量管制應用比較表如表31。

表31　主要非點源模式比較

模式 特性項		SWMM	STORM	AGNPS	ANSWERS	HSPF	VAST	VANTU
適用地區		都市區	都市區	農業區	農業區	都市與非都市	都市與農業區	都市與農業區
模擬時間尺度	單場降雨	✓		✓	✓	✓	✓	✓
	連續模擬	✓	✓			✓		
模擬污染物項目	SS	✓	✓		✓	✓	✓	✓
	BOD	✓	✓			✓	✓	✓
	COD	✓	✓	✓	✓	✓		
	N	✓	✓	✓	✓	✓	✓	✓
	P	✓	✓	✓		✓	✓	
	DO	✓				✓	✓	✓
BMP模擬能力		高	中	中	中	高	高	有
數據及人力需求		高	低	中高	中高	極高	中	中
模式之複雜度		高	中	中	中	高	中	中

(三)绝量管制模式應用

模式應能計算非點源的污染負荷量，並動態的模擬水體之水量和水質，可以評估各種點源和非點污染源管理措施的效應。點污染源的管理措施包括　垃圾管理、廢水處理。非點源污染原的管理包括　土地利用之改變、水土保持、農業耕作管理、肥料施用管理、水邊保護帶之設立、觀光管理、牲畜管理及其他結構性的管理[集水池、場、防砂壩等]等。

非點源最佳化管理措施[BMP]措施模式應能模擬和評估以上之管理方案才為真正绝量管制適用模式，其措施如下

1 經由點源及非點源以模式計算，並檢驗水體水質是否有達到水質標準，如未達到水質標準則採取以下措施

以模式計算點源及非點源減少分配污染負荷量，包括點源一級、二級及三級廢水處理廠及非點源如農地肥料使用、殺菌劑使用情形整理配合，再以模式優選組合，組合可能情形如下

點源

a 一級廢水處理改善

b 二級廢水處理廠改善

c 增設三級廢水處理廠

非點源

a 減少殺菌劑使用量

b 減少農藥使用量

c 增加沉沙池、沉澱池等硬體结構性BMP最佳管理措施

2 由以上負荷減少方案再以模式進行模擬選出數個可行搭配方案且符合水質標準方案再加以選擇。

3 再以成本之方式配合上項已選擇方案，以選擇最佳方案。

4 考慮利益團體，利益團體包括

(1)民眾

(2)環保團體

(3)在地工廠或公司

(4)政府機構

利益團體應參與整個水體保護策略的整組過程，包括 模式篩選及應用，以使各方都能接受模式之應用。

5 以上模式篩選方案配合成本和效益，利益團體之協議，共同考慮才可選擇最可行方案，以使管理方案真正可行。

十、STREAM及ESTURY模式探討及應用

(一)STREAM模式探討及應用

STREAM模式為1960年由美國曼哈頓學院(Manhattan College)所發展(Mueller, 1960)，用以研究Sacramento River之水質，利用質量守衡定律描述物質於河水中之傳輸現象，並以Streeter-Phelps類型之方程式描述水質項目之反應關係，而在一維、定常態及非感潮水體之基本假設下，求解得方程式的解析解，可適用於BOD及DO水質系统之模擬，計算各段落

的CBOD、NBOD、DO deficit（缺氧濃度）及BO濃度。

STREAM模式(Mueller, 1960)，利用質量守衡定律描述物質於河川水體之傳輸現象，以解析法來進行水質模擬，此模式與ESTUARY不同之處乃將BOD分成Nitrogenous BOD(NBOD)及ultimate carbonaceous BOD($CBOD_u$)兩項，並可分開輸入河水與污水之污染源，再曝氣係數亦採用O'Connor-Dobbins方程式，功能上稍較精確且符合實際水質變化狀況。

(二)ESTURY模式探討及應用

ESTURY模式是由美國曼哈頓學院所發展出來之定常態有限差分程式，可用以模擬一維感潮及非感潮河段之物質傳輸，模擬項目包括非保存性物質如BOD、DO，保存性物質如鹽份之分佈。模擬程式係以Fortran-77電腦語言寫成，計算時可同時進行單系統差分模式及雙系統差分模式之演算。

ESTURY模式乃假設每一段落均為完全混和(Complete Mixing)，以有限差分法進行數值分析，在水質參數方面，河川的BOD濃度之去除可以下式表示

$$K_1=K_d+K_3$$

其中，K_d為袪氧係數

K_3為不消耗溶氧之BOD去除係數

此模式僅考慮K_d，即假設大部分的BOD因氧化作用而減少，並以一迴歸式($K_d=1.796\times Q^{0.49}$)及溫度修正式($K_d=K_{d(20℃)}\times 1.047^{(T-20)}$簡化之，再曝氣係數則採用O'Connor-Dobbins方程

式，同時，該模式亦可模擬保存性物質，如鹽類之分佈，其延散參數需由水質資料進行檢定之，應用上相當簡便。

以上兩模式可謂近代水質模式之先驅，於模式建立時便以Sacramento River做分析，且每年在紐約市Manhattan College舉辦講習課程，並以此二模式教授講員，隨著許多功能強大的水質數學模式的快速發展，如QUAL2、WASP系列等，其應用上目前已不多見，Wu-Seng Lung(2000)曾以STREAM模式探討美國Gettysburg的Rock Creek及Virginia州的Roanoke River中DO與CBOD、NBOD間的變化，以作為當地污水處理廠之設計及擴充之參考。

十一、QUAL2E和WASP5模式探討及應用

(一)QUAL2E模式探討及應用

原始的QUAL-II模式乃是在1972年Water Resources Engineers, Inc (WRE)在與U S Enviromental Protection Agency的合同之下更改及擴充由F D Masch and Associates 及Texas Water Development Board (1970)所發展的QUAL-I河川水質模式而建立。並且為反應某些特定使用者的需求而發展了許多不同的版本，例如針對藻類-養份-光合作用之間的相互作用修正的SEMCOG版等。其中，SEMCOG版之QUAL-II後來經由覆審、編輯及修正，並且廣泛被使用，後更經使用者們一連串程式輸入及輸出的修正，將改良過的QUAL-II模式重新命名

為QUAL2E (Brown and Barnwell 1985)。自從QUAL2E發行後，模式亦持續的改良，如加入了河段氣象因子、模式模擬之不確定性分析功能等。本研究所採用之QUAL2E版(3 0版)乃是在Tuft University, Department of Civil Engineering 與 EPA Center for Water Quality Modeling (CWOM), Environmental Research Laboratory, Athens, Georgia之間的合作協議下所發展的，其包括了前一版QUAL2E(2 2版)的變更及廣泛的不確定性分析(UNCAS)與定常態模擬功能。

QUAL2E是一個完整且具彈性的河川水質模式。可依使用者的需求組合模擬十五種水質成份。能模擬的成份有溶氧(Dissolved Oxygen)、生化需氧量(biochemical Oxygen Demand)、溫度、葉綠素a(藻類)、有機氮(Organic Nitrogen)、氨氮(Ammonia)、亞硝酸氮(Nitrite)、硝酸氮(Nitrate)、有機磷(Organic Phosphorus)、溶解磷(Dissolved Phosphorus)、大腸菌(Coliforms)、任何非保存性物質(Arbitrary Nonconservative Constituent)、三種保存性物質(Conservative Constituents)。此模式可模擬充份混合的枝狀河川。其理論假設傳流(Advection)和延散(Dispersion)這兩種主要傳輸方式只在水流的主要流向(河川或運河的順軸)較顯著。它允許多污染物排入(Discharge)、取水(Withdrawal)、支流(Tributary flows)、進流(Inflow)和出流(Outflow)的增量。它還能計算流量補注所需要的稀釋流量以

符合任何預先設定的溶氧量。以水力學上來說，QUAL2E只適用於在模擬時段內之流域水流和流入污染負荷為定常態的狀況下(Steady state)。

QUAL2E主要用來模擬河川水質沿水流方向之變化，其模式應用時，首先將一河川系統根據其水理特性分成數個河段(Reaches)，每一河段具有相同或一致性(Uniformity)的水理特性，即在一河段中的任何斷面之流量、水深、流速均視為相同。每一河段又等分成數個同長的計算單元(Elements)。因此所有河段的計算單元數必需為整數。在QUAL2E中，計算單元分為七種類型

1 源水單元(Headwater element)

2 標準單元(Standard element)

3 匯流點上游之單元(Element just upstream from a junction)

4 匯流點單元(Junction element)

5 河系最下游單元(Last element in system)

6 流入單元(Input element)

7 取水口單元(Withdrawal element)

源水單元為所有的支流、主河川系統之起始，它們必需是源水河段的第一單元。標準單元乃是不符合其餘六種單元類型的單元。因流量增加在所有單元類型中皆被允許，流量增加乃是標準單元中唯一允許的輸入。類型三單元乃是用來指

定在匯流點略上游主幹一個單元。匯流點單元(類型四)則有一個模擬支流進入。單元類型五為河川系統中最後的一個計算單元，類型五單元應該只有一個。類型六與七代表了流入點（污染負荷及未模擬支流）和取水處。而在程式發展中設置了某些單元數目限制。這些限制為

1 河段　最多25段

2 計算單元　每段不超過20個，或總數不超過250個

3 源水單元　最多7個

4 匯流點單元　最多6個

5 流入及流量單元　最多25個

QUAL2E能以定常態(Steady)或動態(Unsteady)水質模式運算，因而為一非常有用的水質規劃工具。當以定常態模式運算時，它可用來研究污染進流負荷對水質的衝擊(量、質與位置)，也可和實地採樣計畫配合使用，來確定非點源污染負荷的量與品質特性。而以動態操作此模式時，使用者可研究每日氣候變化對水質（主要為溶氧與溫度）的影響，並可研究因藻類生長及呼吸而導致的每日溶氧變化。但是，在QUAL2E中無法模擬如源水水流或點源負荷負荷等動態變化之影響。

QUAL2E模式除了可模擬前面所提過之十五種水質項目外，還包括以下的考量與特點

1 考慮藻類、氮、磷、溶氧相互作用。

2 考慮藻類成長速率與光之間的作用。

3 配合河段之氣象條件模擬溫度。

4 不特定非保存性物質。

5 在水理方面可以考慮

  負向流動情況（例如當取水大於流量）。

  沿河段流量漸增的情況。

6 以梯形渠道或階段排入及速度排入曲線來指定渠道水力特性之選項。

7 輸入/輸出可視個人需要採英制或公制。

另外，新版的不確定性分析模式QUAL2E-UNCAS的功能包括下列

1 敏感度分析(Sensitivity analysis)--輸入變數變動的階乘設計組合之選項目。

2 一階誤差分析(First order error analysis)--包括均值敏感度係數矩陣及變異數矩陣成份的輸出。

3 蒙地卡羅模擬(Monte Carlo simulation)--包括輸出變數分佈頻率及統計摘要。

QUAL2E-UNCAS提供模擬者在定常態水質模擬中進行不確定性分析。使用者可依以上這些功能評估模式輸入資料的敏感度和不確定性對模式預測值的影響。模式預估時將不確定性數量化，有助於評估水質的風險。此不確定性分析方法

提供使用者對不確定性最有影響的輸入變數評估，並進行最有效率的資料收集及研究。

(二)WASP5模式探討及應用

WASP (Water Quality Analysis Simulation Program，簡稱WASP)模式是由美國環保署與曼哈頓學院共同研發的水質分析模式加以修改而成(Ambrose et al 1988)。從1970年開始發展至今，中間經過多次的修改，適用於不同水體（包括河川、河口、湖泊及污水處理單元）之水質規劃上，模擬對象由水體之生化需氧量(BOD)、溶氧量(DO)、保存性追蹤劑(conservative tracers)如氯化物、浮游植物、養份，到複雜的毒性物質反應皆有，是一相當完備的模式。本文將採用WASP的最新版本WASP5(Ambrose et al 1993)，介紹其功能及使用程式並進行急水溪的水質模擬。

WASP5模式利用動態分段(dynamic compartment)的方式對模擬水體進行水質模擬。此模式最大的優點是可由使用者依水體情況的需要，決定看是要建立一維、二維或是三維的水體模式，考慮線性或非線性的反應、時變或非時變過程、點源或非點源等，可說是具有非常大的彈性空間。若為時變過程則可指定各輸入資料為時間變數，如延散係數、流量、溫度、污染量、邊界條件及初始條件等。WASP5模式可提供使用者對自然或人為之水體水質污染進行模擬、預測，模擬的

對象包括河川、湖泊、水庫、感潮河川及海岸等水體，而可模擬的項目包括傳統性污染物及毒性物質等。

在WASP5系統中包括了兩個獨立的架構，分別為動態水理模擬(DYNHYD5)及水質模擬(WASP5)，它們可以分別運作，亦可聯合操作。當WASP5在模擬水體分段區間內污染物的傳輸與作用時，可以連結DYNHYD5，計算水體區間的流動情形。依模擬對象又分優養模擬程式(EUTRO5)及毒性物質模擬程式(TOXI5)兩部份。

如2 1的內容所述，WASP在水質模擬分為優養模擬程式(EUTRO5)及毒性模擬程式(TOXI5)。本文在應用上模擬急水溪的DO、BOD及優養，故只對EUTRO5作介紹。

EUTRO5模式可執行湖泊、河川、水庫等多水體的模擬，是一個相當優良的模式，可模擬八大系統(systems)，並可視其模擬對象將其難度分級(complexity level)，可參考表32。由表中知，等級四、五、六的模擬中，八個系統都有模擬，所不同的是，等級四只作簡單的優養模擬，等級五作複雜的模擬，而等級六連水體底床的水生植物也都併入考慮，故有加以區分。模擬的水體最多可分為300個段落(segments)、50個邊界(boundary conditions)、50個污染點(waste loads)、21個參數(parameters)、104個水質常數(constants)及17個時間函數(time functions)。在參數中有溫度、鹽度、底泥需氧量等，而時間函數主要也是配合參數使用，以溫度為例，模擬時間若很長

的話，則溫度變化就不可忽略，此時配合這情況定義一個溫度的時間函數，使溫度成為時間變的函數。水質常數指的是K_2曝氣係數(reaction rate constant)、K_1生化需氧量的耗氧率(BOD deoxygenation rate)等，在模式中的常數，是由使用者自定，有的亦可由模式計算，如K_2曝氣係數，若不輸入模式就會由流量、溫度及水深等，依照各種不同的情況代入不同的公式計算而得。

表32　EYTR05的八十系統及難度分級

系統	簡稱	名稱	難度分級的等級					
			1	2	3	4	5	6
1	NH3	氨氮		×	×	×	×	×
2	NO3	硝酸氮			×	×	×	×
3	PO4	無機磷				×	×	×
4	CHL	藻類				×	×	×
5	CBOD	生化需氧量	×	×	×	×	×	×
6	DO	溶氧	×	×	×	×	×	×
7	ON	有機氮			×	×	×	×
8	OP	有機磷				×	×	×

×代表有模擬的項目

水質模式WASP5依各種不同的水體可作一維、二維及三維的模擬，表面水體變寬大時，可將水體作二維的分段，水體變深時，也可向Z軸方向作分層，當底泥過深時，可分為數層，有支流的河川，也能作分段計算，可以靈活的運用　因有這個靈活特性，所以WASP5可以輕易的用在各種水體上，如河川、湖泊、水庫、海灣等。

(三)WASP、QUAL2E及ESTURY比較

表33為WASP模式與QUAL2E及ESTUARY的簡單比較。在模式理論中WASP與QUAL2E均是以基本物理概念為基礎，故其模擬項目上，故可模擬優養、毒性物質等多項水質濃度，而ESTUARY是以DO、BOD Streeter-Phlps方程式發展出來的數學模式，受理論公式之限制只能模擬DO、BOD兩種水質項目。

表33　WASP與其它水質模式比較表

	WASP	QUAL2E	ESTUARY
模式理論	質量平衡與動量平衡方程式	一維傳流　擴散質量傳輸等式	BO BOD Streeter-Phlps方程式
模擬項目	有EUTRO5和TOXI5可分別模擬優養及毒性物質	可組合模擬15種水質項目	只可模擬DO　BOD兩項
河川分段	可分300個段落	可分25個河段，每個河段不超過20單元	可分99個段落
分段之彈性	可作一　二及三維的計算，故可模擬水庫　河川，河口及海灣	為一維分段，可計算網狀河川，但有匯點限制	不能有匯流點，故網狀河川，要分別模擬
源頭單元	沒有限制	10個	無
匯流點	沒有限制	9個	無
曝氣係數值	模式提供三個公式，亦可自行輸入	模式提供八個公式，亦可自行輸入	模式提供一個公式，亦可自行輸入
動態或定常態計算	動態　定常態	動態　定常態	只能定常態
其它	有DYNHYD5水理模式可配合水質模式作動態模擬	模式中有附風險的程式，可算水質項目的風險	無

在河川分段方面，WASP模式最多可分300個段落(Segments)，其特性在2 4節有說明，本節以說明QUAL2E及ESTUARY，並比較這三個水質模式在分段方面的異同，QUAL2E模式最多可分為25個河段(Reaches)，每一河段具有相同或一致性(Uniformity)的水理特性，即在一河段中的任何斷面之流量

水深、流速均視為相同。每一河段又等分成數個同長的計算單元(Elements)，最多可分為20個單元。而其計算單元又分七種類型。分別為源水單元、標準單元、匯流點上游之單元、匯流點單元、河系最下游單元、流入單元和取水單元。由於QUAL2E對河川計算單元的功能指定分明，因此在網狀河川分段上可以輕易完成，但對三維水體就較無法勝任。而WASP模式並沒有這麼麻煩，每個段落(Segments)，均可有入流、出流、點源、匯流等功能，因此在分段上更加的有彈性，不但可以模擬網狀河川，對二維、三維之水體也是可以輕易分段。Estuary模式跟上兩個模式比起來就顯得遜色許多，Estuary最多只能分為99個段落，且只能作單純河川主流的分段，無法對網狀河川分段，如果是網狀河川，就要分次模擬了。

WASP模式可進行動態的模擬，甚至其水質參數、荷負量、流量等，也是時間函數的型態輸入模式可配合動態模擬，當然只要將所有的參數設成常數，就是定常態模擬了。而QUAL2E雖可然也可進行動態模擬，但是其水質參數、點源荷負均不能以動態變化進行配合，比起WASP可說略微不足了。而ESTUARY無法以動態模擬，只能進行定常態的模擬。

曝氣係數方面，WASP模式提供三個曝氣係數經驗公式，若是使用沒有輸入曝氣係數，則模式會以水深、流速選擇公式計算。QUAL2E模式有八個曝氣係數公式，可由使用者指

定公式計算，如果需要也可以不透過模式計算，直接輸入模式中。ESTUARY模式僅提供一個曝氣公式計算，也可以自行輸入。

另外，新版的QUAL2E-UNCAS模式還有提供敏感度分析、一階誤差分析程式及蒙地卡羅模擬提供模擬者在常態水質模擬中進行不確性分析。使用者可依以上之這些功能評估模式輸入資料的敏感度和不確定性對模式預測值的影響。

WASP與QUAL2E模式是較為複雜的模式，因其強大的計算功能，自然其需要的資料也需較為詳細，而ESTUARY模式是一簡易的模式，只能模擬DO、BOD故且所需要的參數也較少，模式的選擇常視當時情況即使用的需求而定，如果只是要模擬DO、BOD，而水體又不複雜，ESTUARY是不错的模式，若需模擬多種水質項目，則WASP與QUAL2E較能勝任，當水體較不單純時，WASP是較佳的選擇，使用者如需有關水質項目的風險，QUAL2E有提供許多之附屬程式可供計算其風險機率。

十二、AGNPS 和 SWMM 模式探討及應用

(一)AGNPS 模式探討及應用

農業非點源污染模式(Agricultural Non-Point Source Pollution Model, Young, et al, 1995)簡稱為 AGNPS 模式。為 USDA Agricultural Research Service、Minnesota Pollution Control Agency 與 Soil Conservation Service 所共同開發的模式。此模式的發展源於美國聯邦法律規定各州應評估集水區上游地表沖蝕量及其對水質之影響。模式設計的目的主要用以推估逕流性質，特別是沉積物量(Sediment)營養物成分(Neturients)與農藥，經由不斷的發展與更新版本，目前最新的版本為 AGNPS5 00。

AGNPS 屬於單場暴雨事件(single event)、混合參數(lump-sum parameter)與計算污染物負荷(pollutant loading)的模式，此模式屬格網(cell)式模式，適用於模擬單場暴雨事件之非點源污染分析，可模擬集水區及各個網格的土壤流失及總磷與總氮等水質參數，及推估相對的污染潛勢。該模式將集水區分割成一些網格，並給定一個集水區出口。其基本原理是暴雨產生沖蝕及逕流，因而引起流失(loss)及運移(transport)二種作用，AGNPS 藉由分析引起此二大作用之機制，並透過這些實際的區域特性(physical-based)而訂定與水質、水文相關參數，應用於單場暴雨發生下，估算集水區內，非點源產生的污染負荷量，並顯示排出源及污染潛勢的空間分佈。藉由此結果

可用以評估不同土地利用型態的經營價值及對水質之影響程度，進而作為集水區經營規劃與管理之參考依據。

更新功能

以下就 AGNPS5 00 新增功能做一簡要介紹

1　提供三角水文歷線之選項

2　提供 SCS TR55 方法計算尖峰流量

3　考慮營養成分於渠道流中之衰減因素

4　提供 5 種土壤類別供計算沖蝕量

5　使用 Einstein 方法模擬物之傳輸

6　可選某網格來模擬沈積物之累積情形(依 SCS TR55 方法計算)

7　於輸入土壤養分資料中增加了視窗介面

8　可同時輸入肥料氮及磷成份

9　額外沖蝕之土壤特性可另行設定

10 每一貯水池之入滲率可分別設定

11 使用權重式坡度計算尖峰流量

12 使用二種曼寧係數，一用於漫地流，一用於渠道流

13 三角歷線每一段均計算渠道及沈積物運算

14 較多之點源可供選擇

15 飼牧場之氮磷量可分別設定

16 改以 C 語言發展模式

17 貯水池之養分衰減

非點源污染分析－總磷

在非點源污染中，對總磷量進行有效的控制是重要的工作之一，因含磷量是藻類生長的限制因子，且為湖泊水庫水體優養化重要指標之一 AGNPS 5 00 對於總磷量之推估方式分為兩部分，一是可溶性磷，一是附著於沈積物(Sediment)上之磷。

可溶性磷

AGNPS 5 00 對可溶性磷的推估，是依據可溶性磷伴隨逕流在集水區中傳輸的程序，對每一個網格進行演算，將流入目前網格之磷量進行加總，並考慮在流流至網格出口延時期間磷的衰減量以推估可溶性磷量。

附著於沈積物之磷

附著於沈積物中之磷乃是以陸地沈積物產量(Overland phosphorus sediment yield)與溝渠磷產量(Gully phosphorus yield)相加計算之，模式中以產生的沈積物量乘以土壤含氮濃度再乘以氮飽和比率以估算附著於沈積物中之氮量。

非點源污染分析－總氮

水體中含氮量過高，則會增加水處理成本，降低水體用途，氮亦是造成湖泊、水庫優養的因子之一，AGNPS 5 00 對

於總氮的推估和總磷的推估方式類似，亦是根據可溶性氮與附著於沈積物上之氮進行演算，

可溶性氮

AGNPS 5.00 中可溶性氮的演算原理乃是基於可溶性氮伴隨逕流在集水區中傳輸的程序，首先依據 CREAMS 公式計算逕流中含氮，再針對每個網格進行計算，將流入目前網格的氮量進行加總，且考慮流至集水區出口延時期間氮之衰減量估算之。

附著於沈積物之氮

附著於沈積物中之氮乃是以陸地上氮沈積物產量(Overland nitrogen sediment yield)與溝渠氮產量(Gully nitrogen yield)相加計算之，模式中以產生的沈積物量乘以土壤含氮濃度再乘以氮飽和比率以估算附著於沈積物中之氮量。

非點源污染分析－農藥

AGNPS 5.00 模式中對於農藥量之推估是以網格為演算基礎，計算網格內溶解、沈積與滲漏的農藥，並考慮降雨沖刷、逕流、入滲、滲漏、粒子、大小、分配係數等因子以進行演算。

農藥的總量亦分為可溶性農藥與附著於沈積物(Sediment)上之農藥二部分，考慮農藥附著於不同粒子大小及農藥在沈積物與

逕流中重新分配等因子進行估算，摘要其演算程序如下（詳細說明請參見附錄 A3）

1 計算有效農藥量

2 分別計算土壤與植物中的農藥量

3 分別計算殘餘在土壤與植物中的農藥量

4 計算在地面的農華量

5 計算逕流中的農藥量與農藥濃度

6 計算滲漏的農藥量與滲漏的百分比

7 計算可溶性農藥量與可溶性農華濃度

8 計算附著於沉積物上之農藥量、農藥濃度與百分比

(二)SWMM 模式探討及應用

美國環境保護署(U S EPA)發展之都市降雨逕流重理模式(Storm Water Management Model 簡稱 SWMM)，是美加及世界各國廣泛應用於都市暴雨逕流之水文、水力及水質問題的模擬與分析。以下就 SWMM 的發展沿革模式結構及運算功能作簡單介紹，以期模式使用者有初步的完整概念。

1 SWMM 概述

SWMM 是美國環境保護署為都市區域暴雨逕流所發展出來的一套包含水量與水質運算功能豐富的管理模式。第一版 SWMM 是在 1969-1971 年由下列三個單位共同研究發展而成的電腦程式版本

(1) Metealt-Eddy, Inc

(2) University of Florida。

(3) Water Resources Engineers, Inc。

目前以由 Huber and Dickinson, (1988), Roesneretal (1988) 更新改版至第四版(Version 4 0)，但原始版模式運算原理及內容，仍具有參考價值。第一版 SWMM 僅能模擬分析合流式下水道溢流污染問題，第四版 SWMM 之模擬分析功能已擴展至下列各項問題

(1)分流制與合流制下水道之水文水力分析。

(2)都市非點源污染負荷。

(3)都市排水系統設計及未來系統規劃評估。

(4)下水道水質分析

(5)複雜排水系統水理運算。

(6)單場降雨或連續性降雨模擬都市雨水逕流之水量及水質分析。

2 SWMM 模式架構

SWMM 電腦程式是以 FORTRAN 語言撰寫，且 U S EPA 可提供原始程式碼內容供使用者自行改寫以配合實際需求。程式內容是由運算模式、輔助模式及執行組結合而成，如圖 4 所示。

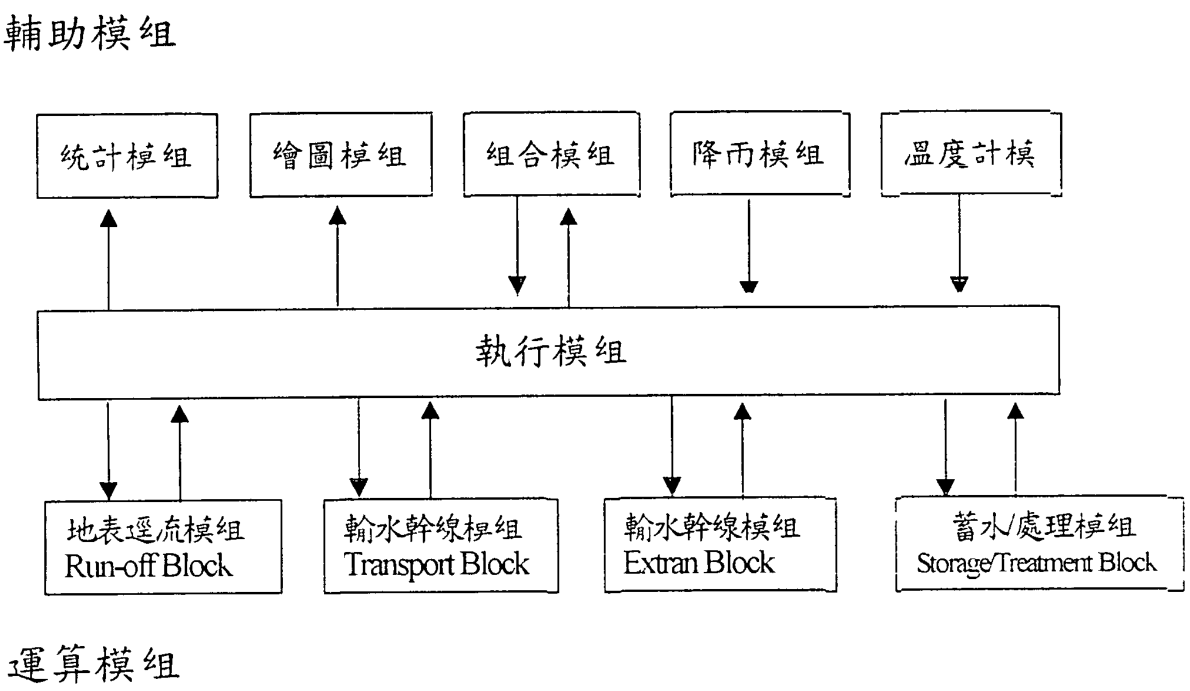


圖 4 SWMM 程式模组架構(Huber and Dickinson 1988)

各項模组之功能如下所述

a 運算模组(Computational Blocks)

(1)地表逕流模组(Run-off Blocks)

利用降雨資料計算出逕流量、污染負荷及水質。

(2)幹線輸水模组(Transport Block)

以運動波方法進行水力演算，並可推算晴天水量及水質問題。

(3)幹線輸水模组(Extran Block)

利用一维 Saint Venant 方程式作水力演算(不包括水質)，因 Extran 模组係以動態流進行水力演算，可模擬流況包括

動態迴水演算

- 迴路型排水網路系統
- 壓力管流演算

(4)蓄水／處理模組(Storage/Treatment Block)

蓄水量演算及處理設施之水質模擬。

程式模組之流量演算特性如表所列。

	地表逕流模組 (Run-off Block)	輸水幹線模組 (Transport Block)	輸水幹線移模組 (Extran Block)
1 流量演算方法	非線性水庫 階梯式管溝	動力波 階梯式管溝	完全方程式 互動性管網
2 計算機費用	低	中	高
3 洪峰歷線衰減	有	有	有
4 洪峰歷線圖	弱	有	有
5 管內貯留	有	有	有
6 迴水及下游控制效應	無	無*	有
7 逆水流況	無	無	有
8 滿流演算	弱	弱	有
9 壓力流況	無	無	有
10 樹枝型管網	有	有	有
11 迴路型管網	無	無	有
12 指定管溝型狀限制數	5	16	8
13 水力設施單元 (如 Pumps、Weirs、Orifices)	WO	PWO	PWO
14 晴天水量及基流演算	部分	有	有
15 污染歷線演算	有	有	無
16 土砂沖淤	無	有	無
17 外部輸入水文歷線/污染歷線資料	無	有	有

*蓄水設施之水平面迴水演算

b　輔助模組(Service Blocks)

(1)繪圖模組(Graph Block)

模式演算結果可利用 Graph 模組在印表機上輸出水文歷線、污染歷線或其它時間序列圖(須有適當的改寫介面，才能在廣泛使用之試算表或圖形軟體輸出 SWMM 演算結果)。

(2)組合模組(Combine Block)

組合模組主要功能是串接前後模組之演算資料及檔案，使演算能順利進行。

(3)降雨模組(Rain Block)

降雨模組可處理長期性之降雨序列資料(以 1 hr 或 15 分鐘為單元)，輸入逕流模組進行連續性模擬演算。

(4)溫度模組(Temp Block)

溫度模組可處理長時間溫度、蒸發量、風速及融雪資料，輸入逕流模組進行演算。

(5)統計模組(Statistic Block)

統計模組有下列運算功能

- 分離連續性降雨模擬結果，形成單場暴雨逕流。
- 依設計規範將暴雨事件排序(例如洪峰量、總逕流量、污染負荷及污染物平均濃度等)。
- 依降雨頻率及重現期距率定逕流及污染物參數。
- 模式演算結果的表格化與圖形化。

- 原始資料之轉化（例如對數轉換）。
- 降雨時序分析。
- EPA SYNOP 程式內定之統計分析功能。

c 執行模組（Eecutive Block）

程式執行模組主要功能是指定檔案之編排資料及程式模組之執行次序。

3 資料輸入與輸出

依據操作手冊(Huber and Dickinson, 1988, Roesneretal 1988)說明，SWMM 模式是依據實例降雨資料進行暴雨逕流演算，有關模式參數資料輸入項目包括

- 降雨（降雨組體圖、臨前狀況）。
- 地貌（地表狀況、地形資料）。
- 氣象（蒸發量、氣溫等　　）。
- 集水區管理狀況。
- 輸水、蓄水及處理設施特性資料。
- 污染歷線及污染負荷量。

SWMM 是由 Runoff、Transport 及 Extran 模組結合成下水道或排水系統之水力與污染演算之核心程式，蓄水／處理模組則是評估分析各項措施與設施在洪水控制與污染防治之成效。SWMM 模式無承受水體水質演算功能，EPA 之暴露評估模式中心(Center for Exposure Assessment Modeling CEAM)改寫

SWMM 之運移模組，加掛 WASP 5 程式，可進行承受水體水質模擬分析。

4 SWMM 之優點缺點

(1)SWMM 模式可配合使用者之需求，容許分離各項模組演算，例如不須考慮逕流模組部分，以外部輸入逕流資料直接做輸水模式演算，而且其輸出結果仍可為一下模組之輸入數據資料，可簡化大型模擬系統之複雜性及率定驗證工作。

(2)SWMM 模式容許選用公制單位或其他慣用單位。

(3)SWMM 模式提供部分參數之預設值，若無預設值之參數，在使用手冊內容中有各項建議值可參考引用。

(5)SWMM 模式之資料輸入與結果輸出頗不友善與不便，輸入之檔案資料係以 ASCII 檔編輯，並以表列格式輸出結果。水文歷線與污染歷線可用行列式印表機輸出，或以表格式資料轉檔進入繪圖軟體處理後再繪圖。上述各種不便之處，經由 US EPA 及使用單位努力，已經可知 GIS 或 CAD 並聯使用，增加 SWMM 之功能性(EPA 在 1993 年以後開始提供 Window 版及 CD-ROM 版)。

(6)(5)SWMM 程式約 1-2 年改版一次，可透過 US EPA 獲得程式檔案與文件，聯絡資料如下

・Model Distribution Coordinator

Center for Exposure Assessment Modeling (CEAM)
U S EPA
960 College Station Road
Athens, Georgia 30605-2720 USA

- Phone (706) 546-3549
- Internet address ftp ftp Epa gov

5 小结

SWMM 模式在美国環保署、顧問公司及學術單位齊力研究發展下，已成為功能齊全且廣泛運用的都市排水系统分析軟體，SWMM 可由 US EPA 電腦開放區中(網路)取得，成本非常低廉（僅收工本費），且程式容易改写介面改善使用性，加上在世界各国已有數以百計之實際範例可供參考，提昇模式之前瞻性及延續性。

十三、GLEAMS 和 HSPF 模式探討及應用

(一) GLEAMS 模式探討及應用

GLEAMS (Groundwater Loading Effects of Agricultural Management, 1993) 模式是由 University of Georgia 的 Bio & Ag Engineering Department 與 USDA-ARS 之 Southeast Watershed Research Lab 所共同發展，此模式之前身為 CREAM 模式。主要應用於小區域 (fildscale)的模擬，可模擬之水質項目包括逕流、沈積物、NO_3-N、NH_4-N、PO_4-P、NH_4-N、總氮、總磷等。

以下數小節就 GLEAMS 模式作一簡要介紹

1 模式介面功能

GLEAMS 模式可於 IBM 相容電腦於 DOS 下作業系統環境下執行，此模式提供一編輯功能，可使用者輸入資料，進行水文、沖蝕、農藥、營養物等參數的編輯，此外模式中並有診斷錯誤之功能、輸入錯誤訊息供指導使用者更正錯誤，令模式模擬之過程更為順利。

2 使用說明及功能簡介

(1) 使用修正型 SCS Curve Method (U S Sonservation Service, 1972) 模擬降雨逕流

(2) 可用 Priestly-Taylor 或 Penman-Monteith 方法(Jesen et 1990)模擬蒸發

(3)更新每項作物之根深(root depth)

(4)侵蝕之模擬加入粒子大小之考量

(5)對氮、磷營養成分模擬因子考慮更為周延

氮之部分包括氨化、硝化、脫硝、固定、消耗、滲漏及逕流等

磷之部分包括礦化、逕流、消耗及滲漏等

(6)加入管理策略因子包括施肥量與種類、灌溉量及耕作因子等

水文因子

GLEAMS 模式中之水文部分對逕流量之推估使用修正型 SCS 曲線碼法推估降雨之逕流，蒸發散潛勢則使用 Penman-Monteith (Jesen et al 1990)，Priestly-Taylor(1972)方法推估。

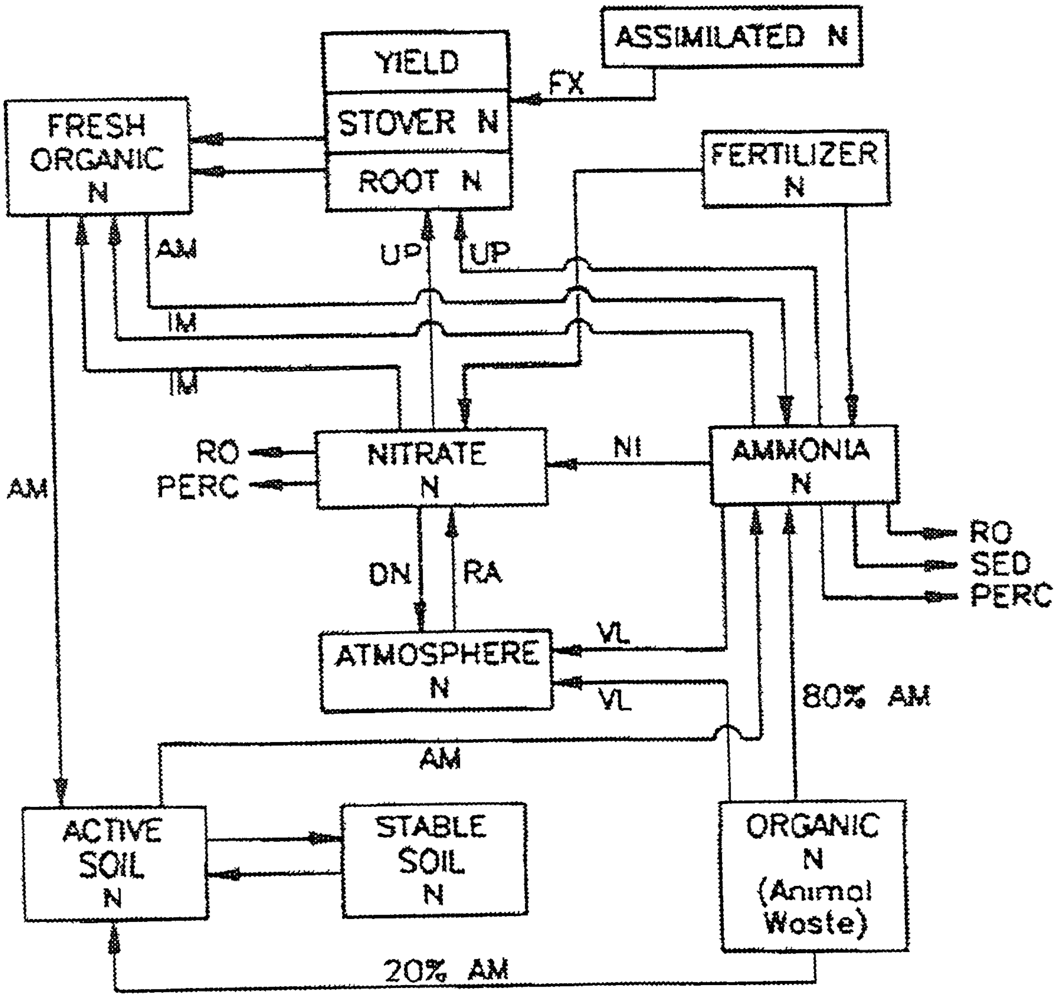
營養鹽成分－氮

GLEAM 模式中對於氮之模擬主要考量因子為氨化(ammonification)、硝化(nitrification)、脫硝作用(denitrification)、揮發(volatization)、吸收(uptake)、固定(fixation)等作用，以經驗或半經驗公式與模式结合而進行模擬，模式中氮之循環圖如圖 5 所示。

營養鹽成分－磷

GLEAM 模式中磷的模擬主要採用 Sharpley 等人(1984)所發展的一長期推估土壤沖蝕與作物性量之模式，此模式冒與 EPIC

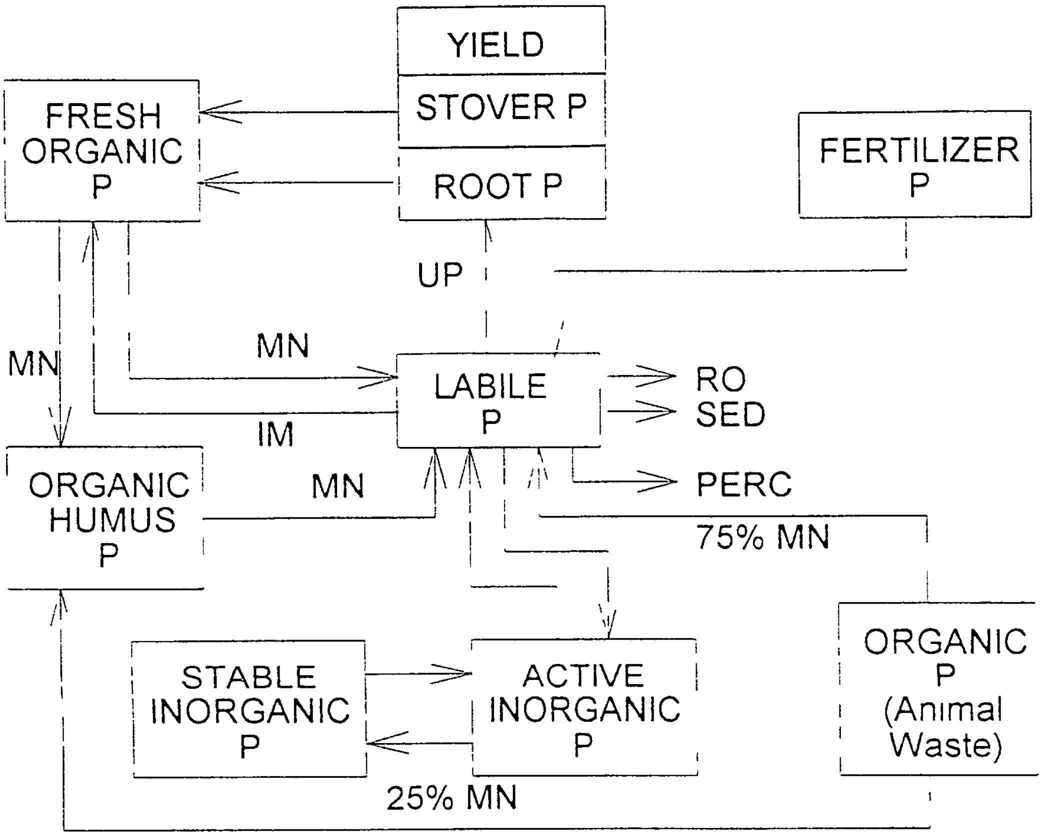
模式(Sharpley & Williams, 1990)合併成功的應用於一大範圍之土壤、作物及氣候區，GLEAMS 模式中則針對此模式並加入礦化作用之修正，GLEAMS 模式中磷的循環圖如圖 6 所示。



AM 氨化 NI 硝化 DN 脫硝 VL 揮發 IM 固定化

UP 吸收 FX 固定

圖 5 GLEAMS 氮循環圖



AM　氨化　NI　硝化　DN　脫硝　VL　揮發 IM　固定化

UP　吸收　FX　固定

圖 6　GLEAMS 磷循環圖

農藥成分

GLEAMS 中農藥成分之模擬主要針對農藥特性、土壤質地、氣候影響、管理策略、表面逕流滲漏與附著等交互作用而進行，模式中亦對施藥後農藥在根深區的質傳進行時間的模擬。

(二)HSPE 模式探討及應用

HSPF (Hydrological Simulation Program Fortran Model)為美國環保護署(USEPA)與 Hydrocomp Inc 所共同發展之模式，為一集合水文、水理、水質於一體之模擬程式。HSPF 發展之目的為模擬集水區之水文、泥砂、殺蟲劑、營養物及其它水質成分，可用於水資源規劃、設計與管理，且可用或外车方法分析水文及水質問題。

1996 年美國環保署所發展之 BASINS(Better Assessment Science Integrating Point and Nonpoint Sources)模式中，將 HSPF 提供了一個簡單的視窗介面。HSPF 可從 BASINS 中執行或獨立執行，根據 BASINS 提供 GIS 圖層資料，對所切割之子集水區執行 HSPF 模式，執行過程會將該子集水區對應之土地利用資料、河川特性資料及點源資料會被擷取整合於模式介面中，如圖 7 所示，另模式所需之氣象資料及相關參數設定值，則須於模式介面中輸入。

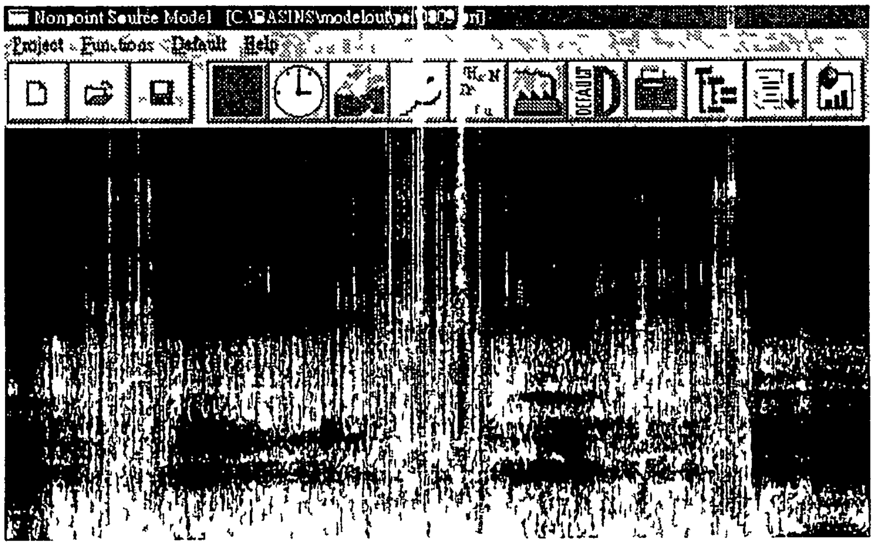


圖 7　HSPF 模式之視窗介面圖

HSPF 為一連續模擬模式，以降雨、溫度、日照強度、土地利用型態、土壤特性和農業耕作方式作為基本輸入資料，根據基本輸入資料，HSPF 最初模擬結果為水量、水質隨時間之變化，從地面經過不同土壤層至地下含水層之傳輸狀況，如圖 8 所示，可預測逕流量、泥砂運移量、營養物、殺蟲劑、毒性物質及其它水質成份的濃度。HSPF 再利用這些結果，考慮河道特性，模擬河道中水量及水質之變化，因此 HSPF 模式可模擬集水區內之水量及水質變化情形。

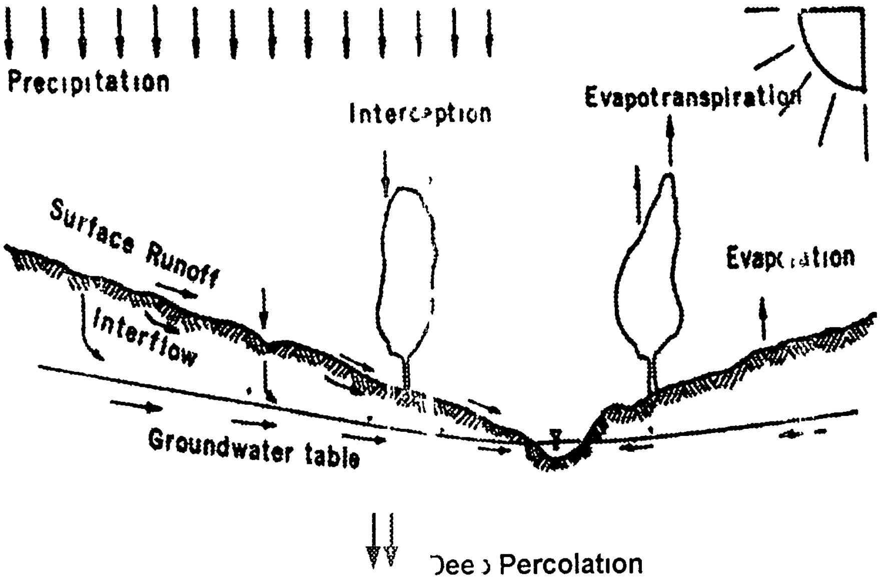


圖 8　水文傳輸圖

國外 Chew 等人(1991)將 HSPF 加以修改和校正應用於 North Reelfoot Creek 流域，對污染控制策略前後之水質變化進行分析。Moore 等人(1992)使用經由 Chew 等修改之模式於美國 North Reelfoot Creek 集水區模擬、評估可執行之最佳管理作業。

十四、BASINS 和 WARMF 模式探討及應用

(一) BASINS 模式探討及應用

BASINS (Better Assessment Science Integrating Point and Nonpoint Sources)為美國環保署(USEPA)發展的集水區多目標環境分析系統，此系統結合地理資訊系統(GIS)、集水區資料庫、及多種水質模擬評估工具，不但美國國內的政府機關、學術單位及民間環境顧問公司廣為使用，也漸漸被其他國家所採用。

為因應美國各州及地方團體以集水區為導向的趨勢，以及1977 年 Clean Water Act 中對水體進行總量管制(total maximum daily load, TMDL)的要求，美國環保署於 1996 年發展 BASINS，以集水區概念為主要架構，將評估 TMDL 所需之點源及非點源污染分析整合成為一完整的系統。BASINS 的三大宗旨包括 (1)落實環境資訊的調查(2)進行環境系統的分析(3)提供評估管理方案的架構。

BASINS 最大特點在於它採整合式(integrating)的系統。傳統集水區評估的方法裡，資料的準備、分析、模式應用及結果輸出評估等步驟常以不同的工具或系統做處理，缺乏整合性且費時，BASINS 克服這些缺點，將集水區資料及評估工具整合於 AreViewGIS 架構下，包括五大項目

※環境資料庫

※水質及點源污染負荷評估工具(TARGET、ASSESS、Data

Mining)

❊工具箱，包括資料匯入、子集水區劃分、資料管理等功能

❊水質模式，包括 NPSM(WinHSPF)、QUAL2E 及 TOXIROUTE

❊資料輸出後置處理工具(GenSen)

BASINS 系統及應用式皆在 Windows 環境下，圖 9 為 BASINS 主介面，介面上方為工具列、左方為資料庫圖層說明、主畫面即為 GIS 圖層展示。GIS 的應用使集水區資料以視覺化呈現，使用者可直接於圖上選取欲模擬的區塊，進入水質模式進行各項模擬或做資料評估，並可提供集水區在 TMDL 方面的分析，從資料的展示、整合、模式模擬、至結果輸出呈現，皆可在 BASINS 系統中完成。

BASINS 包含了 WinHSPF 及 QUAL2E 兩大水質模式，Win HSPF(前身為 HSPF、NPSM 模式)為一非點源污染模式，可根據集水區內水文變化及土地利用的型態連續模擬非點源污染量，QUAL2E 則為模擬點源污染於河川系統中傳輸的河川水質模式。除此之外，美國環保署亦為 BASINS 發展其他輔助工具，如管理程式 WDMUtil 可將氣象資料製做成可供 BASINS 使用之 WDM 檔，集水區切割工具(Watershed Delineation Tool)讓使用者自行將集水區切割成為欲模擬之子集水區，資料匯入工具(Import Tool)可讓使用者將其他 GIS 資料匯入 BASINS，方便模擬工作。

BASINS 有廣大的使用群，因此相關工具及模式發展、更新速度頗快，美國環保署於 2000 年底推出 BASINS3 0 版，除更新模式及輔助工具外，3 0 版改變了對各項工具的管理方式，新發展的 BASINS Extension Manager 功能，將各應用模式、資料管理、集水區評估等功具都視為 BASINS 的”extension”，對工具做更有效的管理，如此使用者在執行 project 時 BASINS 只會 load 所需工具，節省軟硬體空間，程式發展者也易於維護更新各項工具，不需更新整個 BASINS 系統。

BASINS 為一公開軟體，文件、技術支援也相當豐富，網站www.epa.gov/ost/basins/（圖 10）上提供了各式相關資料供使用者參考查詢，值得介紹的是其中的 BASINS Listserver(圖 11)，透過電子郵件，以“討論區”的方式，除了發布 BASINS 相關訊息，更提供使用者之間及使用者及程式技術人員相互討論、集思廣益的機會，尤其是初學者提問題的好地方。

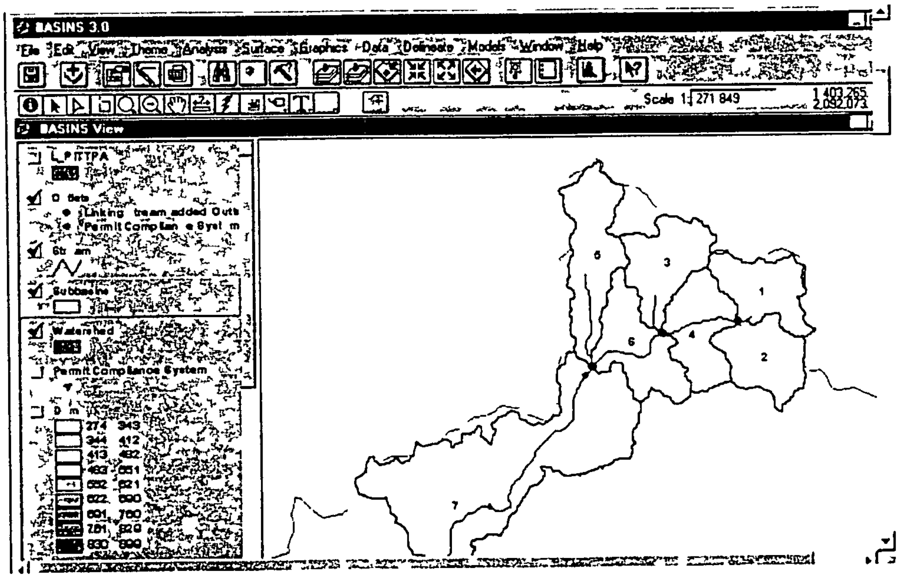
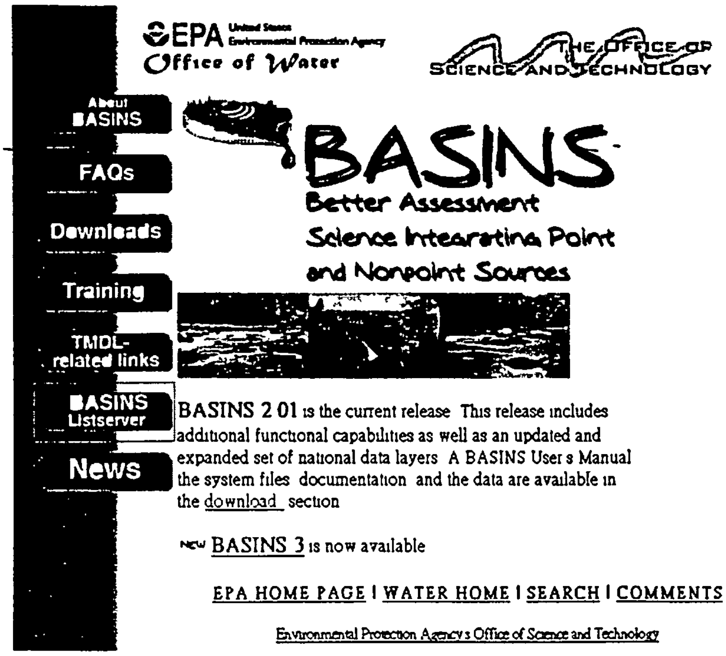


圖 9　BASINS 介面



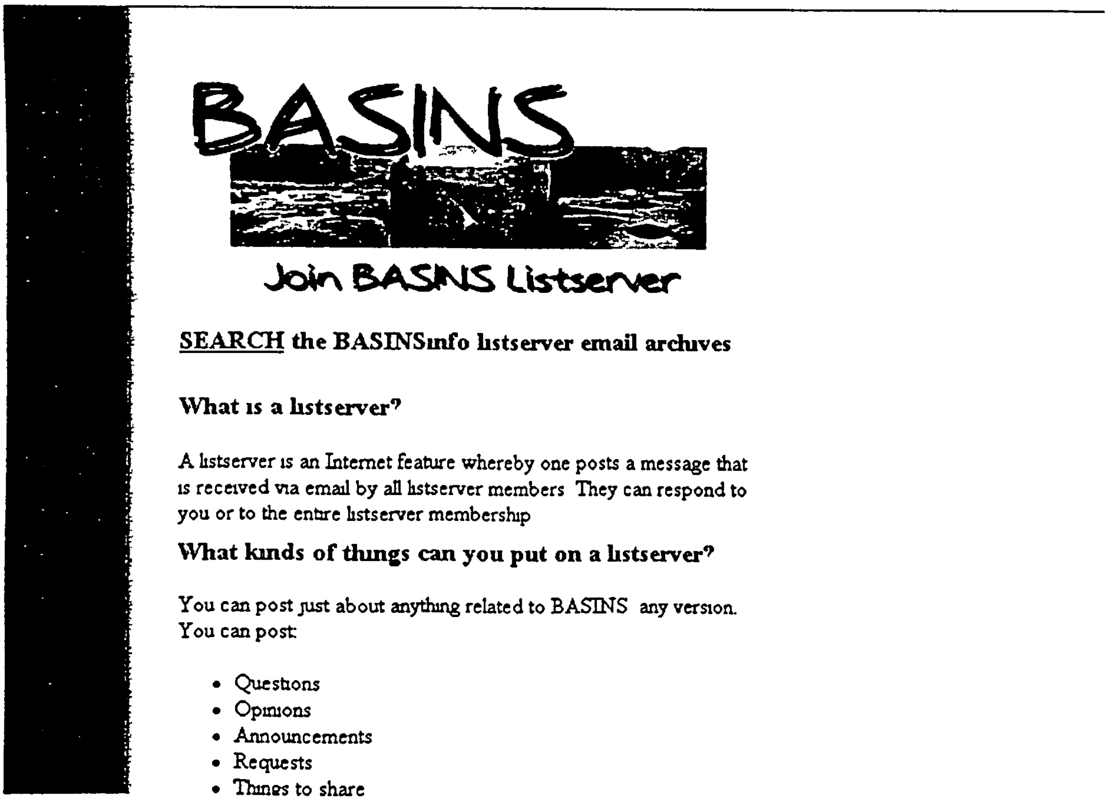
BASINS 2 01 is the current release This release includes additional functional capabilities as well as an updated and expanded set of national data layers A BASINS User s Manual the system files documentation and the data are available in the download section

NEW BASINS 3 is now available

EPA HOME PAGE | WATER HOME | SEARCH | COMMENTS

Environmental Protection Agency s Office of Science and Technology

圖 10 BASINS 網站之網址



SEARCH the BASINSinfo listserver email archives

What is a listserver?

A listserver is an Internet feature whereby one posts a message that is received via email by all listserver members They can respond to you or to the entire listserver membership

What kinds of things can you put on a listserver?

You can post just about anything related to BASINS any version. You can post:

- Questions
- Opinions
- Announcements
- Requests
- Things to share

圖 11 BASINS 提供服務圖

➢應用

BASINS 由美國環保署所發展，提供了完備的美國環境資料庫，因此廣被 BASINS 由美國環保署所發展，提供了完備的美國環境資料庫，因此廣被美國政府機關及學術單位所使用，進行集水區模擬的相關研究，如 Adema(1999)應用 BASINS 於美國維吉尼亞州某集水區，分析不同程度都市化之土地利用對集水區的衝擊。除了集水區水質模擬，BASINS 可進一步應用於集水區總量管制(TMDL)及集水區管理決策，如 Dom et al (2001)以美國馬里蘭州某一集水區為案例，探討城市發展面積與水質改變之關係，說明 BASINS 在集水區水質管理決策上之應用。

由於 BASINS 環境資料庫 水質模式與資料處理評估合一的架構，以及軟體公開 技術支援豐富，BASINS 其他國家的使用者也逐漸增加，常可見到加拿大 印度 台灣等國家的使用者在 BASINS Listserver 討論區與其他使用者交流。

(二)WARMF 模式探討及應用

WARMF 為一整合型之模式，參考模式有美國陸軍工兵團水文工程中心發行的 WQRRS (Water Quality for River-Reservoir System)，美國環保署發行的 WASP (Water Quality Analysis Simulation Program)，在農業集水區方面有美國喬治亞大學發行的 ANSWERS (Areal Nonpoint Source Watershed

Environment Response Simulation Model)，美國農業部發展的 CREAMS(Chemicals, Runoff, and Erosion from Agricultural Management Systems)，和 AGNPS (Agricultural Nonpoint Source Pollution Model)，在都市集水區方面有美國環保署發展的 SWMM (Storm Water Management Model)，包括整個集水區和水庫的有美國環保署發行的 HSPF (The Hydrological Simulation Program-Fortran)和電力研究所發行的 ILWAS (Integrated Lake-Watershed Acidification Study)。

基本上，集水區的水文過程和各種離子的模擬，本模式取長於 ILWAS，土壤的崩離和沉滓在地表的運移取長於 ANSWERS，沉滓在河川的傳送、擴散、沉積和再懸浮參考 HSPF，沉滓95水庫的模擬參考 WQRRS 和 WASP，農藥在植物和土壤的變化過程參考 CREAMS，在河川和水庫的變化參考 WASP。模式的型式是詳細的、決定性的、機械式的、分布參數的、動態的、非線性和模擬性的。模式具有廣泛的分析能力，其本身很複雜，但使用起來並不困難。

WARMF 是一決策支援系統(decision support system, DSS)為設計用在集水區和總量管制。它包括工程、數據總量管制模組，是一完整 Window 之圖形使用者界面系統(graphical user interface, GUI)。

對於 TMDL 發展，使用者能夠遵照一步一步之步驟去達

到 1 水體用途如養殖魚類，可游泳、供水等用途而能達到清水法 303(d)水質限制要求 2 達到水質標準如最少 3 天平均 DO 超過 5mg/l 3 總量管制污染物 4 計算總量管制以調整污染直到達成水質指標。

圖形使用者界面供給緊密界面在使用者與 WARMF 模式和 WARMF 模組之間。經過使用者界面，使用者能進入、評估人及修配輸入數據，操作模擬，展現地理資訊系統圖形和統計輸出，WARMF 模式已有自己的地理資訊系統。它不須 ARCVIEW 去展現輸出模式方法

1 分流域或土地區分，河川分段及水庫分層

2 將土地分成地表迴和土壤分層

3 處理為河川分段或水庫

4 規劃水或水質成分到河川分段經過水源或地下水側流。

5 規劃水或水質成分從河川一段到另一段

6 規劃水域水質成分到一個水庫

7 規劃水或水質成分從一個水庫到河川

8 執行熱堆積計算去決定在河川段面或水庫斷面之水溫

9 考慮水轉向，灌溉

10 考慮土壤腐蝕、沉積侵蝕、化學轉換、藻類生長、藻類營養動力

11 用相同 QVALIE 或 WASPS 之熱堆積和質量平衡方程式

模式將土壤分成 5 層，河川使用為　　，水庫為流　　，在污染源方面考慮點之源、非點源、空氣沉降等，可模擬水質成分為總溶解固體、懸浮固體、溫度、病原菌、殺蟲劑、生化需氧量、溶氧、氮、磷、藻類、鋁、鋅、錳、鐵、硫酸鹽、酸鹼值，其中非點源最佳設計畫使用緩衝帶、滯劑池、沉澱池、沉砂池及衝道掃除等。

應用

1　在加川之 Cata Wba river basin 解決原生動物污染。

2　在加川 Taboe 湖去評估污染交易計畫靠購買灌溉水權增加河川自淨能力以減少非點源負荷。

3　在西維吉尼亞州之 Cheat river Basin 對於黃銅礦污染解決酸鹼值、總鐵鋁、鋅及錳等從酸性礦物排出污染。

4　在賓夕尼亞州 Chartiors creek Basin 解決酸性礦物排出及集合式下水道污染。

5　在科羅拉多州 Dillas Lake 解決生活污染水而使水源可供飲水。

6　應用在田納西州之 Oostanula Creek Basin 中。

表 34 為整合模式 WARMF 與 BASINS 之比較表

表 34 Comparasion of WARMF and BASINS MODEL

	WARMF3 1	BASINS2 0
Design Philosophy	WARMF is a decision support system for the watershed approach It contatins simulation model database built in GIS It provides tools for consensus and TMDL WARMF is designed for use by stakebolders of different backgrounds It makes the translations between water quality and usability and between management plans and model inputs	BASINS 2 is for tegulators to assess the condition of river basins It contains a collection of national databases and water quality models It does not provide a procedure to calculate TMDL Users must find out answers for themselves A stakeholder would not know what to look for and where to find it Regulators are in command and control
Computer Platform	IBM PC With 486 or Pentium processor 16 MBRAM 100 MB hard disk space	IBM PC Pentium processor 64 MB RAM 150 MB hard disk space
Software Requirements	Based on Integrated Lake Watershed Acidification Study (ILWAS) model enhanced with algorithm of ANSWERS	Windows 95/NT Arc View Version 3 0a and Arc View Dialog Designer
Liver Model	ILWAS Enhanced with WASP5	Non point Source Model (NPSM) based on parts of Hydrological Simulation Program-FORTRAN(SHPF)
River Model	ILWAS Enhanced with WASP5	QUAL2E TOXIROUTE NPSM
Lake/Reservoir Model	ILWAS WQRRS CEQUAL-W2	None
Spatial Resolution	Flexible resolution generally applied at 11 digit hydrologic units User can also modify it to a finer resolution	Eight digit hydrologic units by default but may be modified manually by user
Type of simulation	Physically based dynamic simulation normally run with a daily time step for many years	QUAL2E & TOXIROUTE uses only a low flow or a mean flow NPSM can run a dynamic simulation for many years
Fertilizer & cropping	Simulated	Not simulated
Atmospheric deposition	Simulated	Not simulated
Buffer zone	Simulated	Not simulated
Risk Analysis	Can evaluate the risk of failing to achieve the water quality objective of a plan	Not simulated
Pollution Trading	Cost sharing between point and nonpoint	Not simulated
Data Requirements	Digital elevation maps land use soil daily meteorology monthly air quality point source data and model coefficinets	7Q10 USGS Reach File point source data for QUAL2E and TOXIROUTE USGS land use coverage meteorology model coefficients for NPSM
Data Supplied	Data base includes DEM land use point loads meteorology air quality and observed hydrology and water quality This data for the specific river basin is imported from federal state and local sourecs most of which is available over the Intemet or from publisted CDs	Data for all river basins in an EPA region from national database Data for a specific river basin can be sparse Users are cncouraged to import local data for accuracy and resolution Meteorology point source load and observed water quality may not be for the same period
Input/output proccdure	Inpot data can be entered or viewed by couble-clicking at a catchment river or reservoir on the basin map Comparison of model results and observed data can be viewed by double-clicking at a monitioring location on the basin map	NPSM, QUAL2E TOXIROUTE have their own input procedures using menus and buttons

十五、總量管制水質模式之建立

本總量管制首先訂定模式建立之流程如附圖 12，再分別介紹流程中之步驟。

(一)河川水質模式建立之流程

河川水質模式流程，內容共包括七個步驟

1 水質模擬項目之確定

2 水體特性之判斷

3 資料收集

4 水質模式之評選

5 河川分段

6 參數之選取

7 模式之率定

本模式以模擬 BOD-DO 模式為主，但是上述之七個步驟，卻是建立河川水質模式之通用流程，亦即如優氧模式或毒性物質模式，通常均可依此一流程予以建立，只是每個步驟之內容（作法）不同而已。

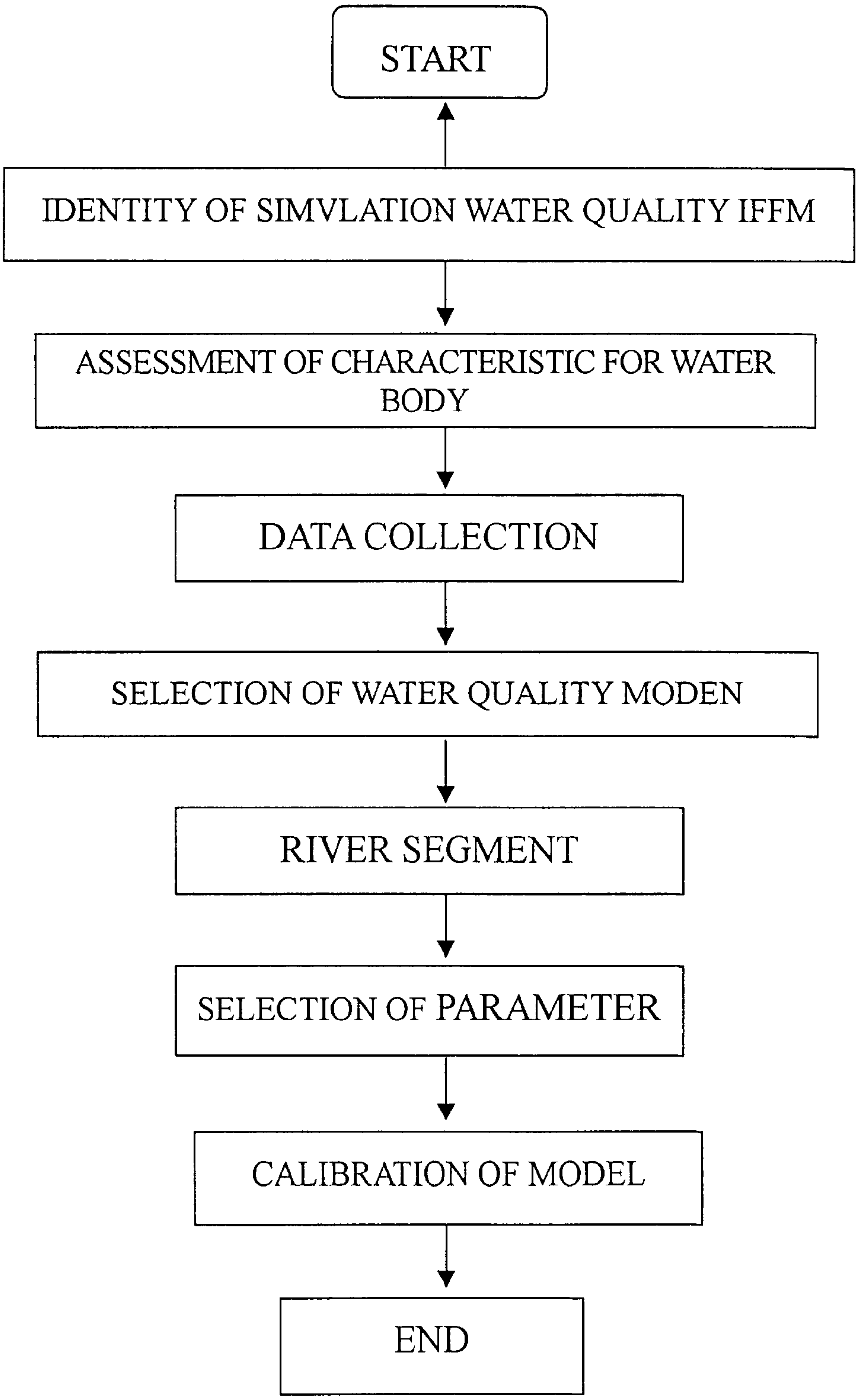


圖 12 ERCTION OF WATER QUALITY MODEL

(二)水質模擬項目之確定

確定水質模擬項目是建立水質模式的第一個步驟，目的是在協助評選出適當的水體水質模式。由於水質模式開發時各有不同程度的學理假設，所以沒有任何一個水質模式對各種情況之水體均適合模擬，況且有些時候因資料缺乏或模擬目的之考量，以太過於複雜的水質模式來解決單純的水質問題，反而只有徒困擾、事倍功半。進行水質模式模擬之前，首先確定要模擬之水質項目，才可衡量相關資料是否足夠，進而考慮採用模式架構的複雜性，例如模式可模擬的水體維度、水質系統，以及是否具備水理模擬能力等。最後才能由諸多模式中，評選得最適合的水質模式，所以確定水質模擬項目是評選水質模式的首要程序。

如何確定水質模擬項目，其實並無一定的準則，因為以往進行水質模擬乃先有水質模式，再依模式可模擬項目收集資料，模擬後判定模式對水體的適用性，如果模式率定被使用者接受，則水質模擬項目即是模式可模擬之水質項目。此種反向的操作乃著眼於建立模式，模擬項目之確定只是一種型式，對於以往水質模式較少而選擇空間較小的情況下，此種過程並沒有錯誤。

以下四點，作為確定水質模擬項目之程序

1 水質問題之確認

確認水質問題才能瞭解影響之因素有那些。通常欲進行水質模擬乃水體出現問題，例如溶氧過低魚、蝦及藻類死亡、水生態改變乃優氧化等。另外，可能水體未受到破壞或污染，為了防止未來污染問題之發生，而就特殊目的進行水質模擬。

2 瞭解水體用途

瞭解水體用途才能知道規定的水質標準。大體而言，水體用途可區分為給水用水、遊憩用水、農漁產用水及生態保育用水等四類，表 35 有更詳細地將此四類水體用途所包含的用水項目列出，每一種水體用途其水質標準並不相同，所以必須先瞭解水體用途，才能知道規定的水質標準。

3 瞭解水質標準

根據水質標準所規定的水質項目，作為水質模式之模擬項目。每一個水體用途分類各有其水質項目之要求標準，水體要能滿足水質標準，才能不妨害其正常之功能。

4 確定水質模擬項目

水質標準所規定的水質項目可能有多個，此時可依水質資料及問題之重點選定水質模擬項目。

(三)水體特性之判斷

一般水體可區分為河川、湖泊、水庫、河口、海岸及地下水等，每一種水體的水理及水質特性不盡相同，水質模擬前應先予以瞭解，對模式之評選及參數之選取會有幫助。河

川可分為水理及水質加以探討。

表 35 水體用途及用水項目

水體用途	用水項目
給水	家庭用水(飲料、沐浴、洗滌、廁所)工業用水(鍋爐、製造、冷卻)、公共用水(清洗街道、公廁、消防)政府機關及公司行號用水、農業灌溉用水
遊憩	游泳、划船、垂釣、滑水、水上摩托車、艇等水上親水活動，旅館、遊樂區之遊客餐飲及廁所用水，環境綠化及景觀維護用水
漁、農產用水	淡、鹹水之貝類及漁業養殖用水，雞、鴨、牛、羊等禽畜之畜牧用水
生態保育用水	水鳥、候鳥、魚類、貝類及蝦蟹類之運動棲息，紅樹林、水筆仔等珍貴植物保育之用水

1.河川水理特性分析

河川水理特性包括流量、流速、水深、坡降、潮汐及斷面變化等。流量是最主要的水理特性，因為流速、水深、潮汐水位及渠道斷面等均與其相關，如果河川之平均流量或枯流量較小，代表其稀釋作用能力較弱，故可承受的污染量較低。流速、水深及坡降與水體的混合作用有關，這些水理參數可直接影響水質特性，例如污染物的分解作用、再曝氣作用及光合作用等。感潮河川受海水漲退潮作用之影響，流速及水位之變化較非感潮河川複雜，鹽水之密度高於淡水，可能造成水質之分層現象。此外，大河川之主、支流交匯處，可能會有特殊流況之發生，所以均要特別注

意加以考量。

針對水體的水理特性作研判，主要有以下四個考量的要點，瞭解後對評選水質模式有很大的幫助

(1)水理資料是否充分

若流量、流速、水深及斷面等資料充分，水質模式可考量不需具備水理運算功能，而直接利用現成資料計算水質參數，或是依模式要求之資料輸入，便可模擬河川水質。

(2)河段是否感潮

感潮河川之水理及水質特性較為複雜，所以有一些水質模式不能應用於感潮河川，又如果水理及水質特性隨時間之變化不大，則可考量進行潮平均之模擬，而不需採用動態水質模式。

(3)河水是否分層

此點乃係指模式維度之考量，分層包括垂直方向或水平方向。以感潮河段為例，海水與淡水密度之不同，使水質可能有垂直方向的分層分佈，此時為了確實掌握水質狀況，至少要採用二維水質模式。

(4)主、支流交匯情況

主、支流交匯處流況較複雜，例如可能有水平方向的二次流產生，此時便可考量用水平二維水質模式，有時更

需採用具水理計算功能之模式。

2 河川水質特性分析

水質特性包括污染物種類、藻類生長、硝化作用及底泥成份等。雖然水質模式依模擬系統可分成溶氧模式、優養模式、毒性物質模式及地下水質模式等四種，但有一些模式可同時模擬兩種以上水質系統，所以應視水質特性選擇便捷的水質模式。基本上，為了便於決定水質參數以及評選水質模式，水體水質特性有必要依以下四點進行研判

(1)水質資料是否充分

水質模擬時，除了決定水質參數必須要有可靠的水質資料外，越複雜的模式進行率定，其所要求的資料就越多，所以水質資料是否充分，乃評選水質模式之要點。例如以動態水質模式進行感潮河川之水質模擬，必須要有時變的水質資料，以配合潮汐水理資料給定，模擬結果才能掌握住水質特性，如果資料不夠則應避免採用動態模式。

(2)藻類生長情形

河水中藻類(葉綠素)之多寡，除可用以研判水生植物之光合作用產氧量是否要考量外，某些地區甚至可能需進行優養模擬，所以此點可作為評選水質模式之依據。

(3)硝化作用是否明顯

硝化作用之過程會消耗溶氧，如果硝化作用很明顯，則必須妥善考量給定硝化參數。

(4)瞭解底泥的成份

底泥需氧量之量測並不簡單，經由底泥成份之瞭解，除可決定底泥需氧量外，底泥中重金屬或毒性物質之含量，有助於提早發現一些尚未發生的水質問題。

(四)資料收集

在水質模式選定前，收集資料的目的是供評選水質模式之用，水質模式選定後，資料收集主要是為了提供建立水質模式之需，所以資料收集乃建立水質模式過程中，一個重要且隨時應進行的步驟。根據本研究所訂定之流程，水質模式之評選視水質模擬項目及水體特性而定，所以為協助評選得適當的水質模式，可由第(二)及(三)節瞭解要收集的資料有那些。

大致上，所需要收集的資料歸類為以下四項

1 溫度資料

乃係指水溫或氣溫資料。水質應用上定 20℃為標準水溫，許多水質特性會隨水溫改變，所以要利用水溫資料來修正水質參數。如果無實測水溫資料，氣溫資料可作為一個給定之參考基準。

2 水理資料

包括流量、水深、流速、渠道坡度、通水斷面積及朝夕流況等資料。流量資料主要是可用來推估設計流量，並可藉由迴歸分析求得其他水理參數，以供作水理模式之輸入資料。水質模擬時，水深、流速、渠道坡度及通水斷面積主要是用來推估水質參數，對於不具水理運算能力之水質模式，這些水理參數被要求直接輸入以計算水質參數，或是使用者計算得水質參數後，再輸入水質模式。朝夕流況之水流較複雜，許多公式之選用必須視感潮與否而定，所以必須加以觀測。另外，河水水是否分層及主支流交匯之流況，亦要一併予以觀測及注意。

3 水質資料

水質參數、係數及實測水質資料之收集，乃為進行水質模擬不可缺乏的步驟。本研究有介紹如何量測及計算水質參數與係數，但若以往有作過相關研究之資料，可收集以作為參考，主要的 BOD-DO 模式參數包括延散係數、再曝氣係數、底泥需氧量及去氧係數等。實測水質資料主要供模式率定之用，收集的資料內容視選定的水質模式而定，未確定水質模式之前，平時可依水質標準所規定的水質項目，建立完整的水質資料庫以供隨時取用。

4 污染源資料

水質模式要求輸入污染源資料，主要包括污水流量及污

染負荷量。以 BOD-DO 模式而言，污染源可能來自家庭、都市污水、工業廢水或農業放流水等，這些資料反應出水體承受之污染特性。通常模式所指的污染負荷為污染源中的 BOD 含量，若有考慮水體的硝化作用，則污染負荷應再包括污染源中的氨氮含量。污染源有分點源及非點源兩種，一般水質模式主要可模擬點源污染，若欲考量非點污染，則評選時要留意模式是否具備此功能。

(五)水質模式之評選

自然界水體之運移及物化反應過程複雜，會隨時間及空間之不同而有所差異，所以水體特性無法完全以方程式代表，故於水質模式開發時，通常會依水體之特性及模擬的水質項目，作一些學理上的假設以簡化模式架構。由於每個模式可模擬的水體特性及水質項目不盡相同，所以進行水質模前，必須先就水體特性、水質模擬項目及資料之多寡等因素加以考量，選定適合的水質模式再予以應用，如此才可避免於實際模擬時遇到各種難題。

先前的三個步驟主要的目的在協助評選水質模式，所以在此將之綜合歸納，得到以下七點可作為評選水質模式之依據。

1 可模擬項目之確認

確認要模擬的水質項目是否包括於模式之可模擬項目之

中，何如 BOD、DO、藻類、硝化作用及養份(氮及磷系統)等。。

2 是否具有水理計算功能

如果已有完整的水質資料，可直接輸入水質模式或另進行水理模擬，則水質模式可不用具備水理計算能力。

3 適用水體之考量

考量模式可模擬之水體，例如湖泊、水庫、海口等。至扵模式是否要求可適用扵感潮河川，視模擬水體之特性或模擬目的而定。

4 維度的考量

模擬維度越多需要輸入的資料越多，模式架構及輸入格式越複雜，視水體特性及模擬目的考量模擬之維度。

5 污染源之特性考量

主要指模式對點源與非點源污染之模擬功能。大部分水質模式直接輸入污染物負荷，以考量點源之污染，但支流排入之污染因隨其流量而變，如果以點源的方式考量，無法反應出其污染量隨時間變化之特性，故對於大河川之支流流量大時，應以輸入污染物濃度考量為較佳，至扵模式內部其實仍以污染之量考量。

6 繪圖功能之考量

為了便扵模式率及觀察模擬結果，模式最好具有繪圖輸

出功能，但此點非屬必要。

7 模式操作之難易度

許多模式由國外引進，可能無詳細的使用手冊或中文說明書，而造成對模式之不瞭解及參數給定的困擾。另外，模式是否提供單位換算功能，而不需使用者自行逐一轉換再輸入，此點有必要加以考量。

(六)河川分段

天然河川渠道變化極不規則，水質模式為便於運算處理，必須將模擬河段依水理、水質特性及模擬目的予以分段，才可使各段落之特性行為能為水理及水質參數所代表。當河道流況特殊(如橋樑、彎道或陡坡)或有大支流匯入時，對水質模擬之結果會有很大的影響。當進行河川水質規劃時，利用水質模式之目的為模擬河川水質，以瞭解河川水質之現況及未來變化。因此，對於有污染源排入、水質變化特殊、水質資料較完整及易於觀測與特別目的要求之地點應予以區分，以便於模擬所得之資料，能確實提供作分析及決策之用。

一般而言，水質模擬為求模擬結果與真實水質狀況易於比較，可依下列原則對河道進行分段

1 水理特性有顯著變化之處。

2 主、交匯之處。

3 橋梁或有實測水質資料之觀測點。

4 污染源排入之處。

5 每個段落之長度不宜過長，通常盡量不超過 2 公里，尤其下游河段應在 1 公里以內。

河道劃分完成後，配合推估得之排入污染負荷量及污水流量，在實測或設計流量與溫度下進行水質模擬，模擬結果除可作為驗證參數之外，亦可瞭解、預測水體水質狀況與特性。

(七)參數之選取

進行水質模擬時，主要輸入的參數包括設計溫度、設計流量、飽和溶氧量及水質參數與係數。一般而言，參數之選取著眼於必須有完整的資料，再依據水體特性選用推算公式，才能得到理想的參數值。

1 設計溫度

設計溫度之決定應視模擬目的而定，率定模式時則輸入實測水溫。以河川 DO 濃度而言，規劃及防治河川水質污染時，設計溫度越高代表水質之要求較高。設計溫度沒有固定的決定準則，通常視水溫記錄或氣溫資料而定，一般大約為 26℃或 27℃。

2 設計流量

美國設計流量有採 Q75 及 7Q10 兩種，不管採用何

種設計流量，詳細而完整的流量記錄不可缺少，尤其不具備水理計算功能的水質模式，設計流量通常左右模擬結果。

3 飽和溶氧量

飽和溶氧量與水溫、河水鹽度及水面壓力有關，資料量測及收集時，應注意將此三者納入考量。由於大部分污染以河川下游較嚴重，而河川下游靠近海平面，所以壓力可以假設等於一大氣壓，至於水溫及河水鹽度因量測容易，所以一般水質資料通常都有包含，所以飽和溶氧量之計算較無問題。雖然並非所有水質模式均要求輸入飽和溶氧量，但由於其直接影響 DO 模擬之結果，所以要確實推算不可任意給定。

4 水質參數

在水質模式中，水質參數代表水體水質之行為，所以如果能正確的估算得水質參數值，模擬之結果將可充分反應出水質特性。

(八)模式之率定

水質模式選定後，依所需之參數及資料輸入模式，必須再經模式率定才可實地應用，所以模式率定是建立水質模式的最後一個步驟。簡言之，模式率定乃係指藉由調整水質參數或係數，使實測水質資料與模擬結果比較，兩者

差異小而模擬結果可被接受之過程。

一般水質模式之率定方法，有優選法及試誤法兩種

1 優選法

此法須水質模式另配合優選模式才可進行，優選模式中有定義一作業函數(performance function)，此函數代表優選效益值，當效益值達到要求之標準，水質模式才算率定完成。作業函數由使用者依認定的效益訂定，例如模擬值與各觀測點實測值之總差異量，可被定為一種負面的效益，作業函數即以數學式用來表示其間之關係，此負面的效益若小至某種程度，而可為使用者所接受，則水質模式即可告率定完畢。

優選法率定模式之過程，乃先將水質資料及推算得到之水質參數輸入水質模式，當水質模式模擬後輸出結果，由優選模式來判斷是否滿足標的效益，若不滿足則調整模式參數繼續重新模擬，如此循環直至達到要求之效益為止。此法除定義作業變數不易外，如何結合水質模式及調整水質參數，均為不易解決的問題，所以應用上較少使用。

2 試誤法

試誤法率定水質參數，可簡單分為以下六個步驟

(1)確定率定之水質參數

針對模擬項目之不同，模式所需率定之參數對模擬結果之重要性亦有輕重之分，尤其各種水體之水質特性變化極大，某些參數可能在模擬時不予以考慮，所以就不需加以率定，此對模式率定過程而言，可節省許多時間及收集資料所耗費之人力。

(2)決定初始水質參數

由經現場或實驗室量測進而推算得之水質參數，因模式架構及理論假設之關係，輸入模式後模擬結果與實測資料不夠接近，故才有模式率定之必要。而因模式乃是在符合現狀況下開發出來的，所以現場量測得之水質參數應與適當的模式參數值相差不多，否則應代表模式不適用，故初始水質參數其實即現場或實驗量測得之水質參數。

(3)選取率定模式之實測水質資料

如果模擬區域之實測水質資料充分，則可選擇多場資料用以確實率定參數，但因流況的變異性及採樣的時機與誤差等因素，並非所有實測水質資料均適宜用來率定模式。由於集污區污染流達量乃根據各項污染原推估得到，如果此污染流達量推估正確，則沿模擬河段之污染流達量，排入水體應會形成濃度高低不等的分佈。污染流量達量輸入模式後，各段落濃度視其污

染負荷量與上游濃度而定，所以模擬結果會與污染流達量濃度分佈一致。因此，實測水質資料之濃度分佈，若與污染流達量濃度分佈之趨勢相同，才是適當的率定模式之實測水質資料，反之，則不應選定以率定模式。然而，如果大部份實測水質資料之濃度分佈趨勢，均與污染流達量濃度分佈不一致，則可能污染流達量之推估有誤。

(4)進行水質參數之敏感度測試

由於操作者可能不具理論背景，所以當模式參數過多時，無法有效及快速地決定要調整那一個水質參數，使模擬結果能迅速逼近實測資料，故率定模式前可先進行水質參數之敏感度測試，以瞭解參數對模擬結果之敏感程度，以作為率定模式時調整參數之依據。水質參數之敏感度，乃係指增加或減少參數某定量百分比(通常為10%或20 %)，觀測模擬項目之變化尺度，由於每次只調整單一參數，所以由變化尺度之大小，即可瞭解各參數對模擬結果之敏感程度。

(5)檢定水質參數

初始水質參數輸入模式後，可進行各種流況之水質項目模擬，模擬之結果並與相同流況之實測水質資料比較，以調整找到適當的各段落水質參數。水質參數之檢定主要係調整參數，使模擬結果逼近實測水質資料，

由於用以率定模式之實測水質資料有先經過篩選，所以模擬結果與實測水質資料之分佈應趨勢會一致，故可由上游向下游針對較敏感的參數進行調整，使模擬結果迅速逼近實測水質資料，再作其他參數之細部調整，最後找到適當的各段水質參數。

(6)驗證水質參數

當經由參數之檢定使模擬結果逼近實測水質資料後，並非代表所有流況之水質，都可以利用此組檢定得之參數加以模擬，必須另外找到數場實測水質資料來進行水質參數驗證。驗證水質參數之目的，乃希望率定後之參數可適合於各種流況之水質模擬，所以並非檢定之結果良好即可，有時最佳之水質參數組合，其檢定之結果並非最好。而唯有同時通過參數檢定與驗證過程，參數才可算完成率定。

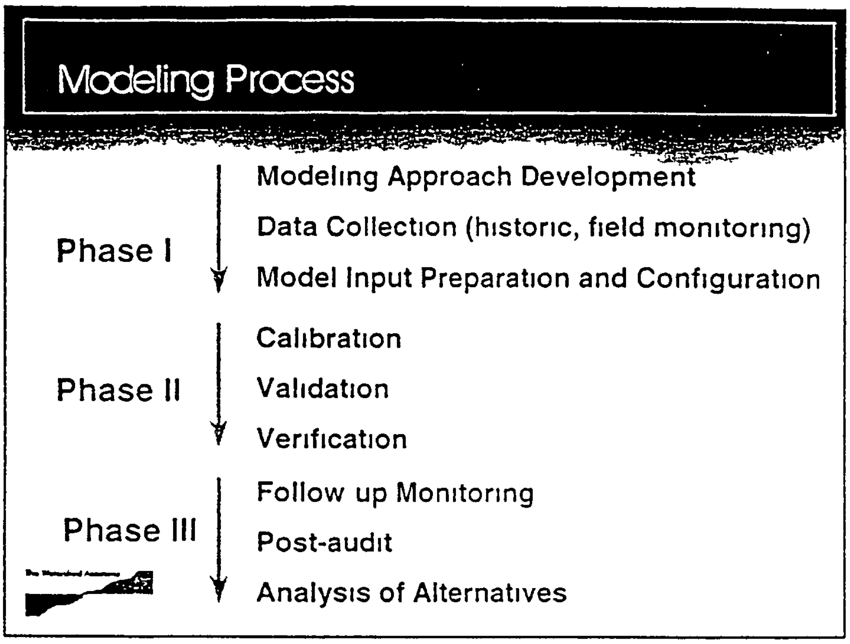
模式率定過程其實要靠理論觀念及經驗，對於 BOD-DO 模式應用於台灣地區，可先自行模擬鹽份分佈(保存性物質)，以率定得河川延散係數，再曝氣係數、底泥需氧量及光合作用產氧量通常直接以適合的公式計算，而最後便只有去氧係數需率定。至於參數率定時要增加或減少，就必須靠理論觀念判斷，例如 DO 模擬結果過低，可提高再曝氣係數或減少去氧係數，以提升 DO 模擬值。

十六、模式應用程序

模式應用程序分三階段，第一階段為模式方法發展、資料收集及模式輸出及結構，第二階段為模式校正、驗正及修正，第三階段為監測、事後審核使用替代方案分析，模式應用程序如圖 13，在發展模式方法考慮因素為模式發展目的，模式技巧的知識，了解被模擬問題，模式需那些資訊來配合，模式所需資料庫運用數據是否足夠。

模式之應用程序分四大類 1 控制程序 2 時間尺度 3 空間尺度 4 模式檢試，模式應用組成架構如圖 14，其中控制程序如圖 15，包括模入資料如時間系列空間和景觀、承受水體、數學應算如景觀、集水區模式及承受水體模式輸出資料包括時間序列等。時間尺寸要在集水區模式選擇具代表性時間間段如乾季、濕季及重要時點，另要選擇具代表性時間階段，如長期平均、短期日和小時平均及相對比較分析。時間尺寸度在承受水體模式模式亦要選擇具代表性時間，另選擇具代表性階段為考慮模式步驟如優養化及沈澱機制及能相對比較分析。高間尺寸考慮為流域負荷評估計畫發展及完成，污染控制設計，河川水質傷害及分析及水資源最佳化管理完成信用。空間尺度在集水區模式分為如個集水區加以水資源最佳化管理措施如圖 16。

圖 13　模式應用程序



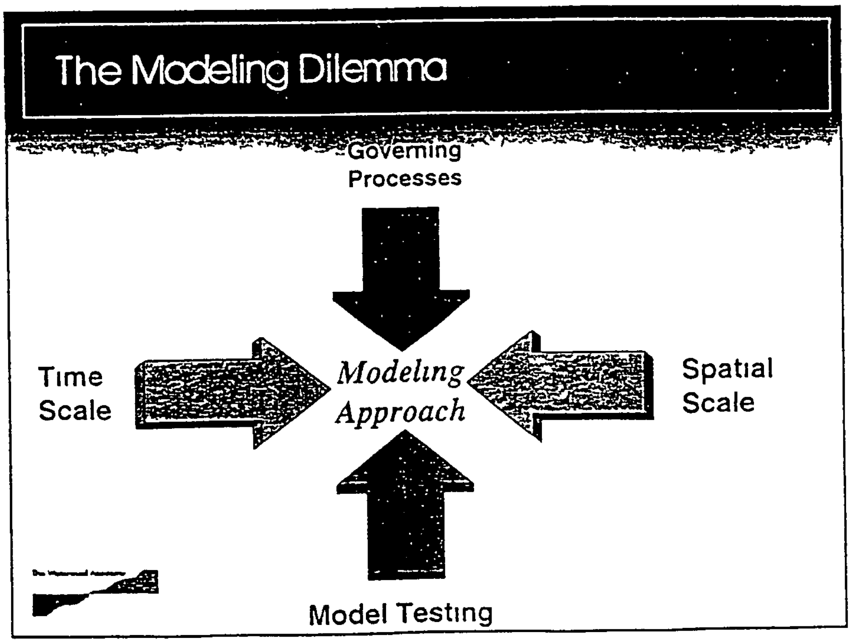
Modeling Process

Phase I
- Modeling Approach Development
- Data Collection (historic, field monitoring)
- Model Input Preparation and Configuration

Phase II
- Calibration
- Validation
- Verification

Phase III
- Follow up Monitoring
- Post-audit
- Analysis of Alternatives

圖 14 模式组成架構



The Modeling Dilemma

Governing Processes

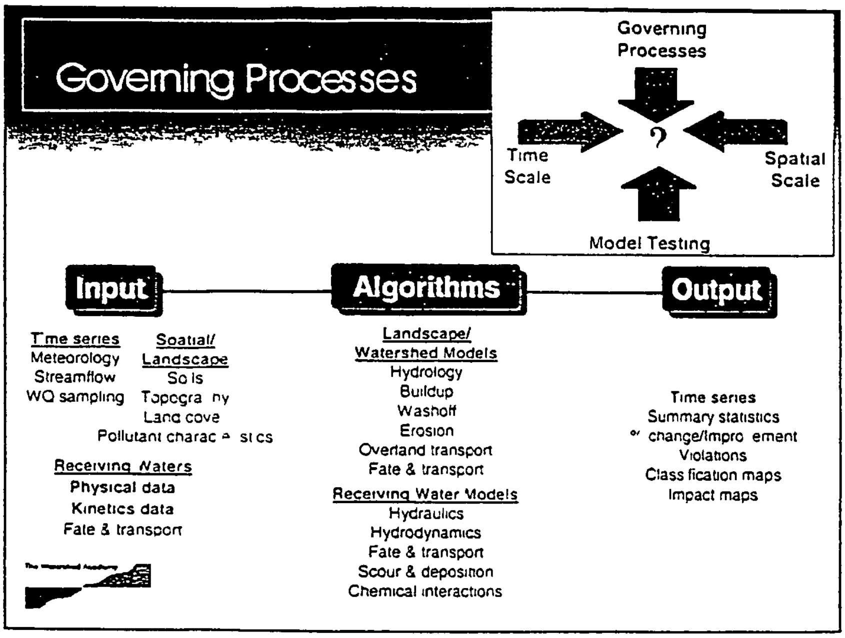
Time Scale

Modeling Approach

Spatial Scale

Model Testing

圖 15　模式控制程序



Governing Processes

Governing Processes

Time Scale

?

Spatial Scale

Model Testing

Input — **Algorithms** — **Output**

Input

Time series
- Meteorology
- Streamflow
- WQ sampling

Spatial/ Landscape
- Soils
- Topography
- Land cover
- Pollutant characteristics

Receiving Waters
- Physical data
- Kinetics data
- Fate & transport

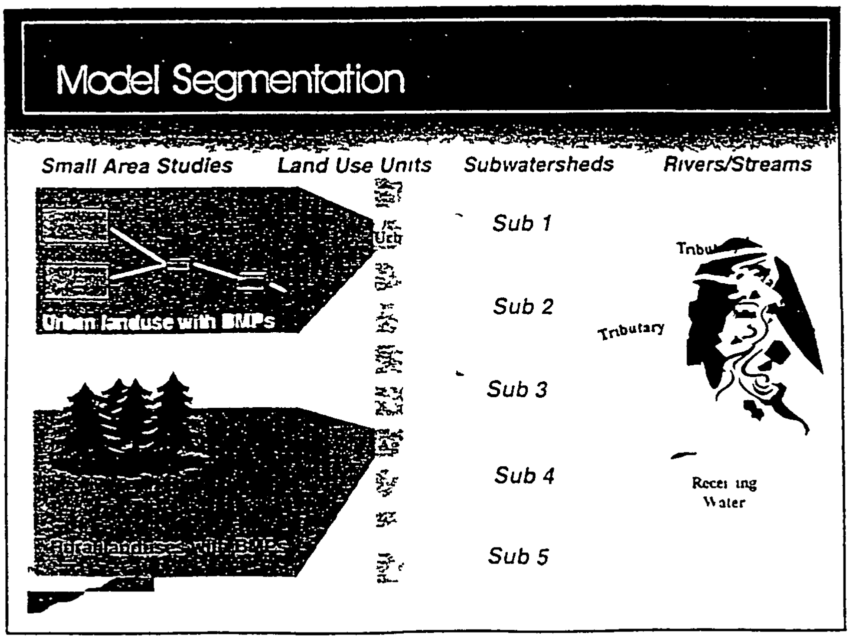
Algorithms

Landscape/ Watershed Models
- Hydrology
- Buildup
- Washoff
- Erosion
- Overland transport
- Fate & transport

Receiving Water Models
- Hydraulics
- Hydrodynamics
- Fate & transport
- Scour & deposition
- Chemical interactions

Output
- Time series
- Summary statistics
- % change/improvement
- Violations
- Classification maps
- Impact maps

圖 16　集水區模式分為數個次集水圖關係圖



Model Segmentation

Small Area Studies

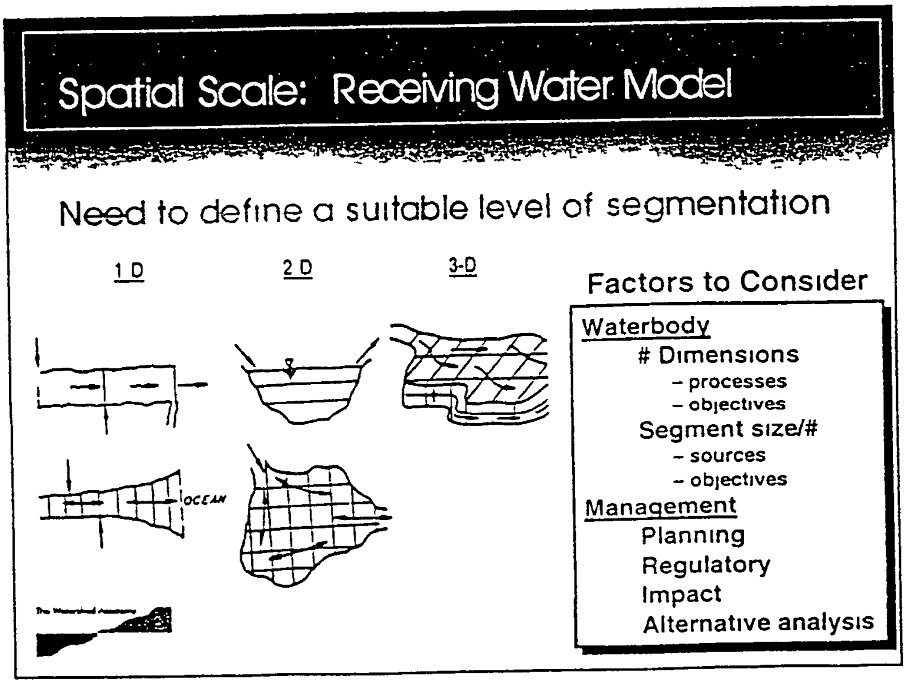
Land Use Units

Subwatersheds

Rivers/Streams

空間尺度在承受水體模式可分為 1 2 3 模式應用如圖 17，維模式應用為較少之橫向之變化，較少或無垂直方向分層，無死角循環區域，適用在有較好混合河川。二維模式應用為有方向變化，較少橫方向分層，複雜水平循環模型，適用在較淺混合良好湖或河口。三維模式應用為有橫向方變化，垂直分層存在，複雜水平及垂直循環，要適當水平與垂直數據供模式校正之用，適用在深湖泊寬廣混合較差海口。

圖 17　1 2 3 維模式應用



Spatial Scale: Receiving Water Model

Need to define a suitable level of segmentation

Factors to Consider

Waterbody
- \# Dimensions
  - \- processes
  - \- objectives
- Segment size/#
  - \- sources
  - \- objectives

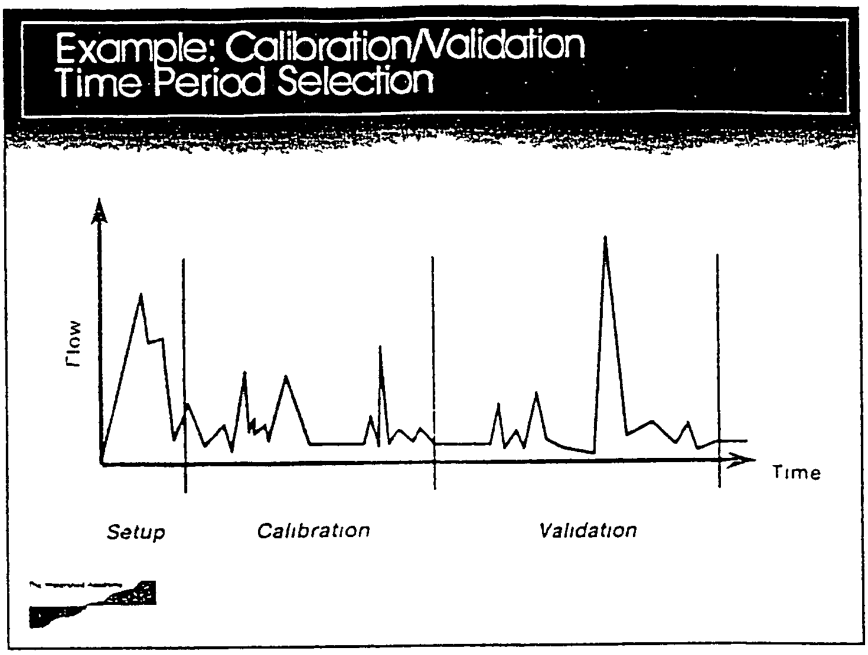
Management
- Planning
- Regulatory
- Impact
- Alternative analysis

數據收據包括 1 地理位置數據如河川流域網、土地利用、土壤分類、集水區邊界地形圖、水質及生物監測站位置、氣象站位置、設備位置圖、廢棄物位置、開挖或廢棄礦產設備，水庫位置 2 監測數據如河川橫切面率光曲線、水庫體積、表面積、排放特性及水深量測、流量連續資料及尖峰資料，氣象連續記錄、降雨、溫度、風速、濕度、露點、蒸發、太陽輻射、水質之化學、生物及沉澱數據等，3 土地行為及活動如水點之源最佳化管理，廢棄物棄置、農業行為像穀物、牲畜、肥料經營、殺蟲劑利用、自然資源像木材砍伐、探礦等。

去支持校正建議所需監測包括測站空間分布，瞬間的監測、河川流量、優養化模式校正資料、病原模式校正資料、溫度模擬資料、沉澱傳輸模擬資料。

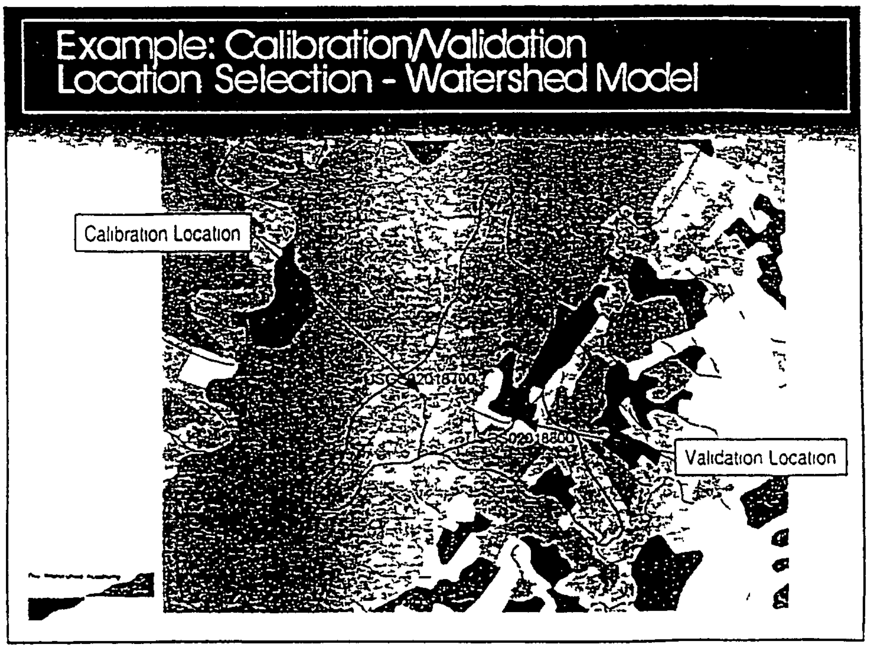
模式測式中校正所需資料為可利用監測資料，有關之區域，水文範圍及與水質相關情形，對驗正所需資料為獨立時間區間、不同位置，可利用監測資料校正所驗與時間關係如圖 18，校正與驗證地點選擇圖如圖 19，模式結構在集水區模式考慮關鍵因素為適當排水面積，經過研究面積水文情形變化土地利用分類排列，模式結構水利變化如圖 20，模式結構土地利用理想狀況之技巧為監測獨立土地利用子集水區，從附近監測資料利用，從一地區外插至另一地區（根據不透水區域），模式結構理想狀況如圖 21。

圖 18　模式校正與驗正時間關係圖



Example: Calibration/Validation
Time Period Selection

圖 19　模式校正與驗證地點排列



Example: Calibration/Validation
Location Selection - Watershed Model

圖 20　模式结構水利變化圖

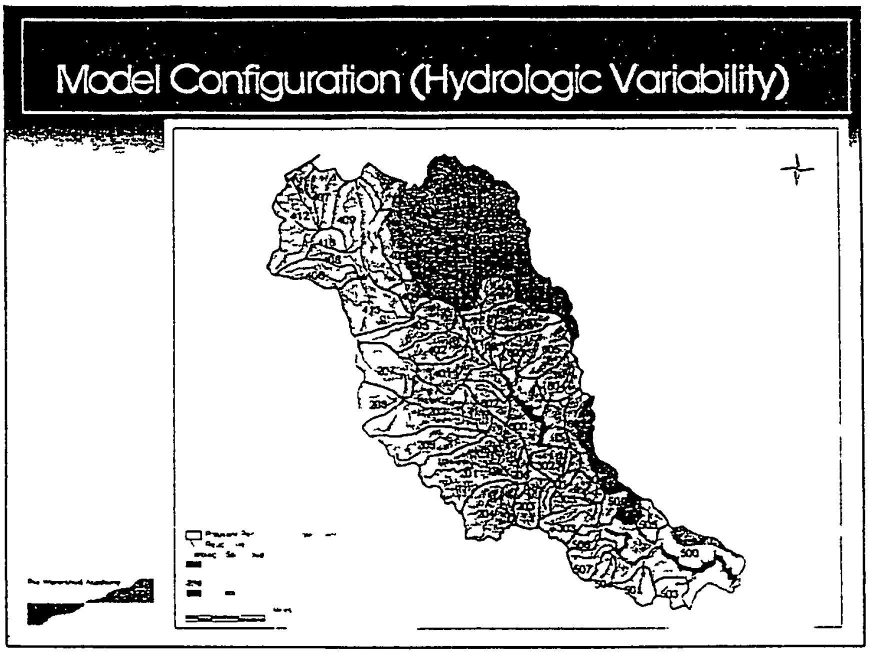
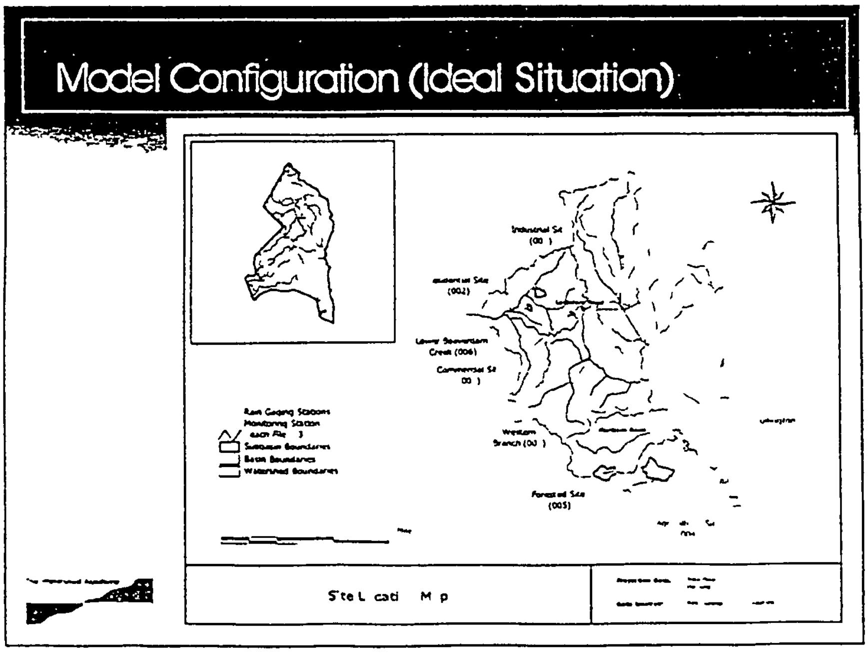
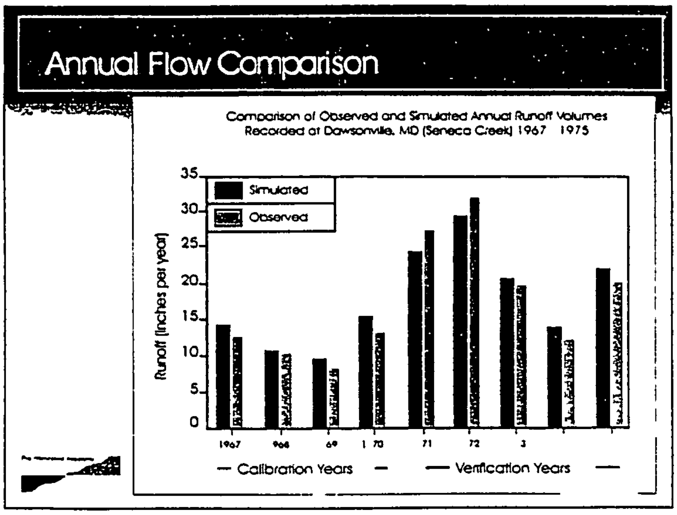

Model Configuration (Hydrologic Variability)

圖 21　模式结構理想狀况


Model Configuration (Ideal Situation)

模式中流量校正分析考慮因素包括每年水平衡，季節分佈暴币流量，基礎流量及水文成分分佈，其中比較方法包括，時間比較校正曲線如年干均、月干均、星期干均、日干均及小時干均、流量一頻率曲線圖、線型迴歸方程序式曲線及统計比較。干年均校正圖如圖 22，小時校正圖如圖 23，流量一頻率校正圖如圖 24，月及星期線型迴歸校正曲線如圖 25。

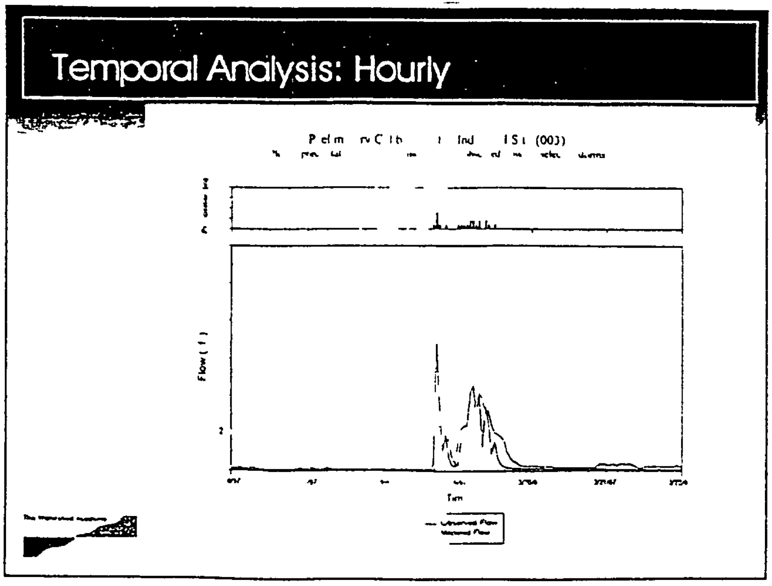
圖 22　模式年干均校正圖



Annual Flow Comparison

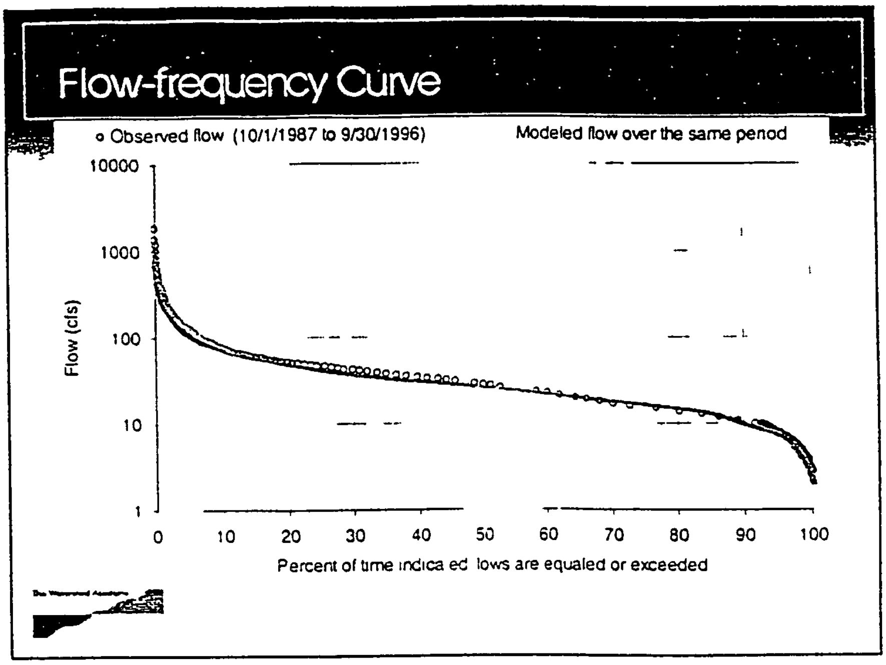
Comparison of Observed and Simulated Annual Runoff Volumes Recorded at Dawsonville, MD (Seneca Creek) 1967 1975

圖 23　模式小時干均校正圖



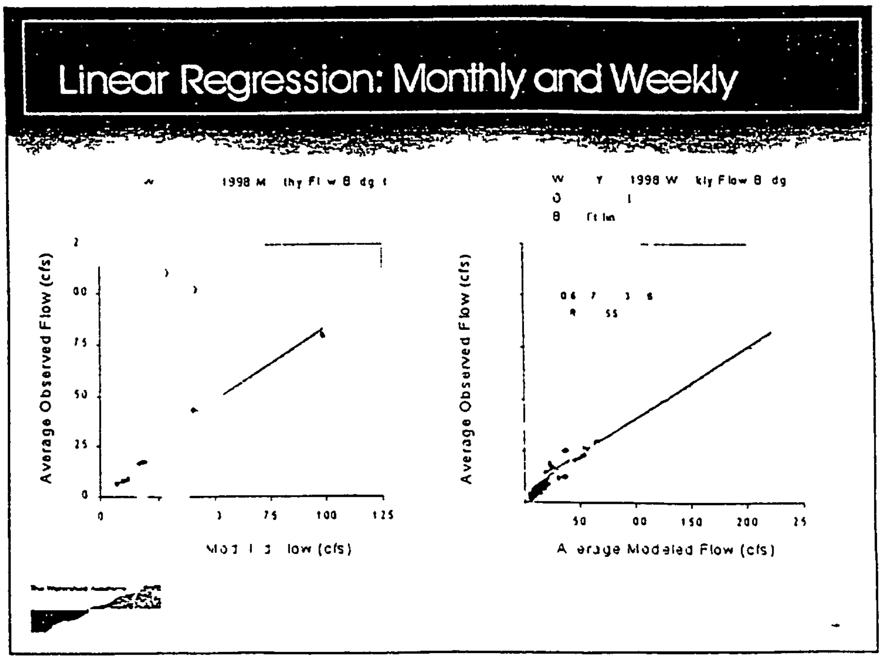
Temporal Analysis: Hourly

圖 24　模式流量一頻率校正圖



Flow-frequency Curve

圖 25　模式月平均及星期平均線性迴歸



Linear Regression: Monthly and Weekly

水文校正時經常出現不準確情形如圖 26，解決對策包括 1 從代表性氣象站取得降雨資料 2 從特殊期間仔細審查降雨和流量資料。

圖 26　水文校正因雨量站不具代表性之不準確圖

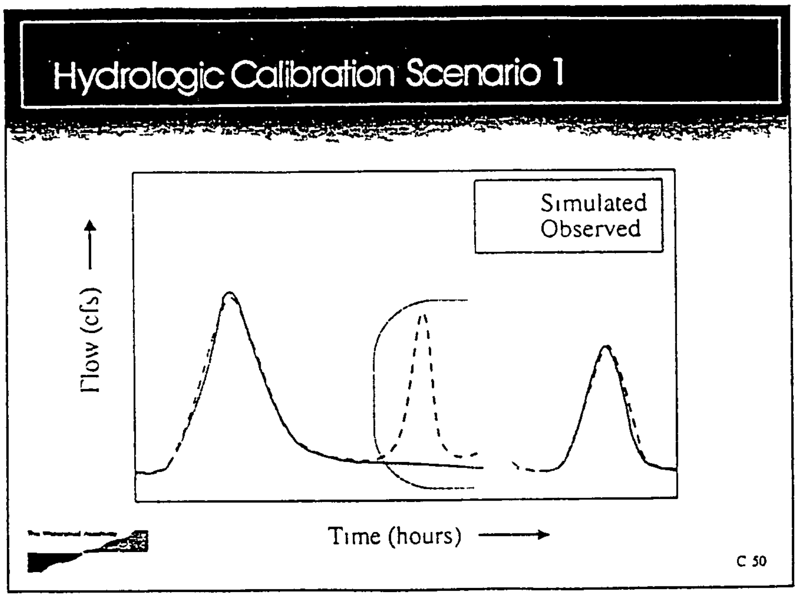


圖 27 為較少蒸發傳輸導致模式不準確性，解決之法為 1 增加深層滲透損失 2 增加蒸發傳輸 3 檢查流量轉換並未包括在此模式中。

圖 27 模式校正之水文蒸發傳輸較少不準確圖

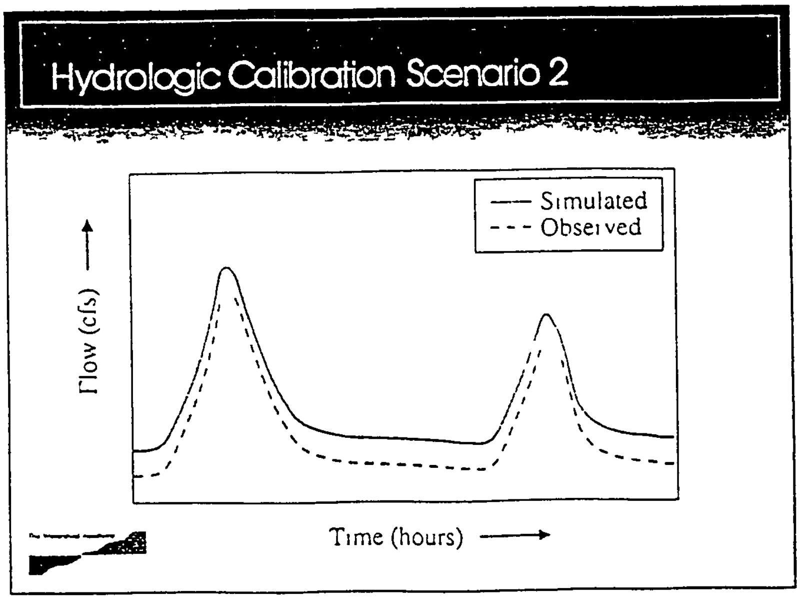


圖 28 為地面坡度非準確之校正偏差圖，解決對策包括調整地面流量之坡度 2 調整地面粗糙係數

圖 28　水質模式校正因地面坡度偏差之不準確圖

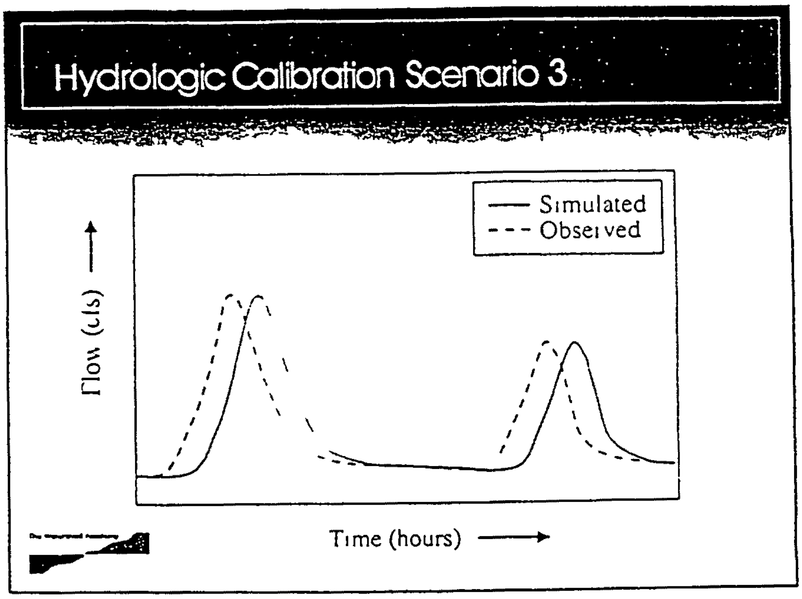
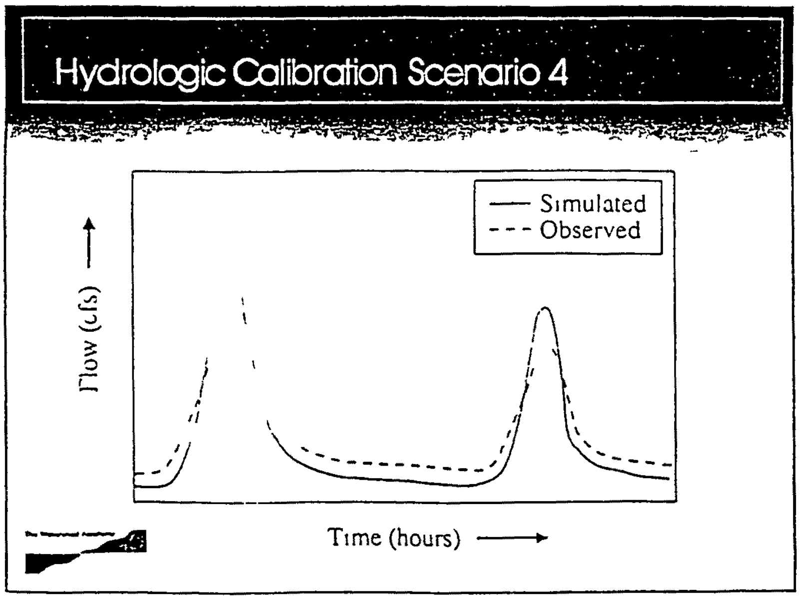


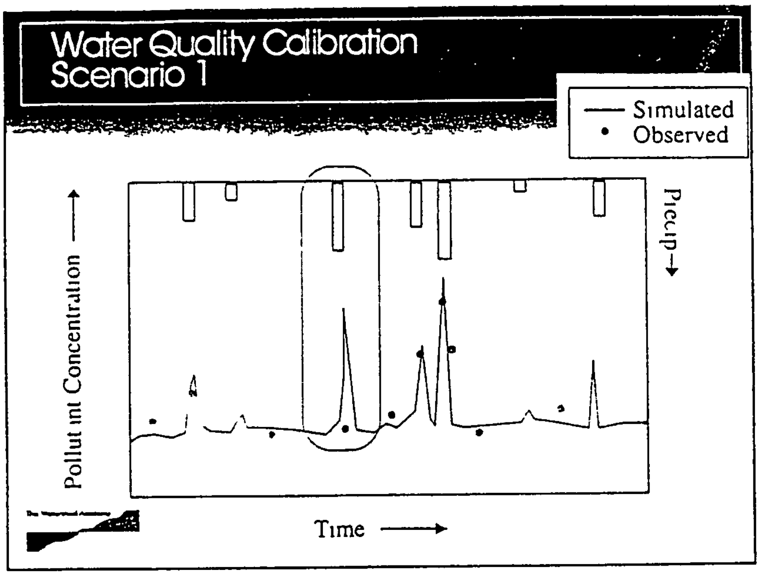
圖 29 為太高表面逕流之校正偏差圖，解決對策包括 1 調整滲透 2 調整混合流。

圖 29　水質模式因太高表面逕流之不準確圖



水質校正分析考慮因素為年平均負荷，季節變化在暴雨時之濃度，混合流和地下水成分，來源供獻，相同應用流量校正作比較方法，圖 30 為模式於暴雨時未反應於集水區中，解決對策為確實比較模擬與觀察之流量。

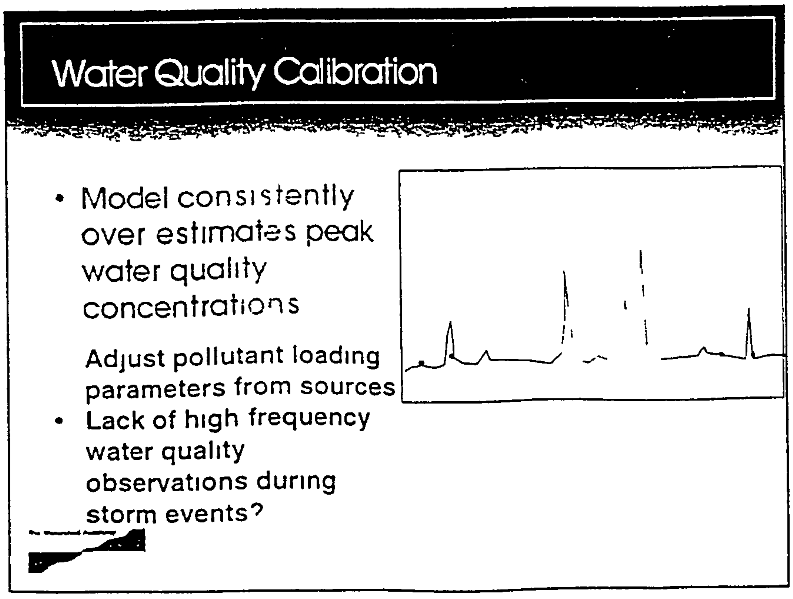
圖 30　水質模式校正因暴雨期未反應之不準確圖



Water Quality Calibration
Scenario 1

圖 31 為模式連續高估尖峰時水質濃度，解決對策為從來源調整污染負荷參數。

圖 31　水質模式連續高估尖峰時水質濃度不準確圖



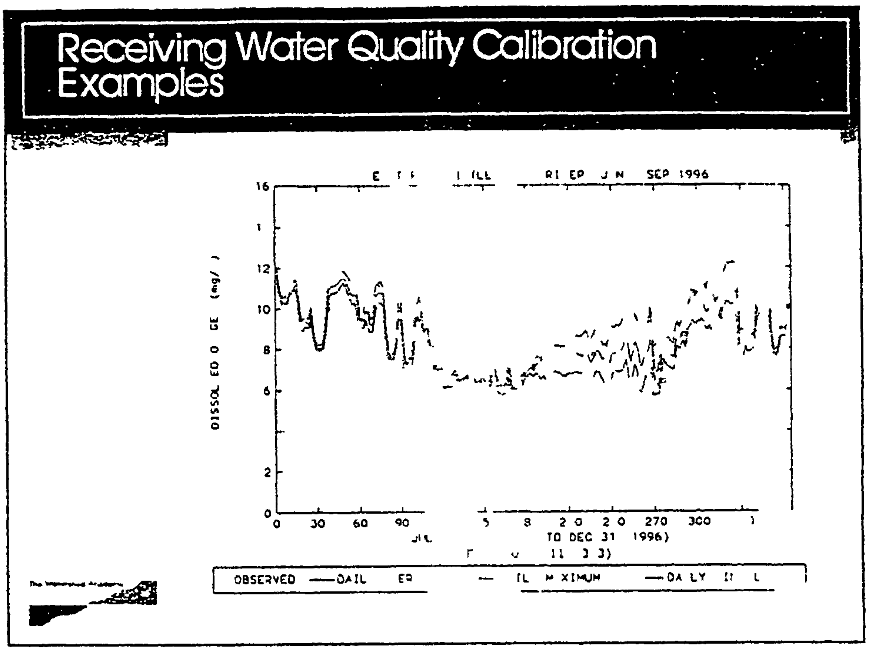
Water Quality Calibration

- Model consistently over estimates peak water quality concentrations

  Adjust pollutant loading parameters from sources
- Lack of high frequency water quality observations during storm events?

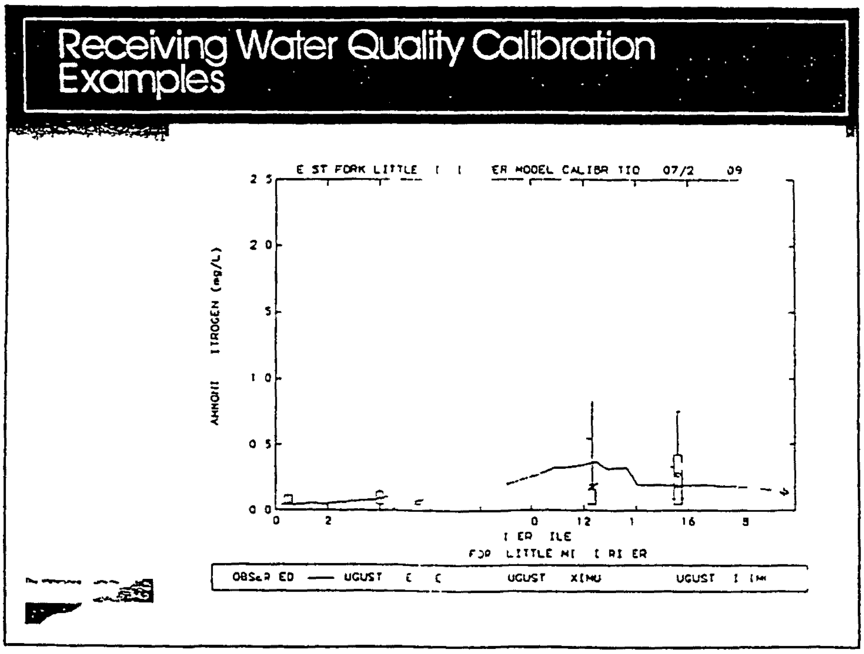
圖 32，33 分別為模式模擬水質濃度圖

圖 32　模式模擬溶氧濃度圖



Receiving Water Quality Calibration Examples

圖 33　模式模擬氨氮濃度圖



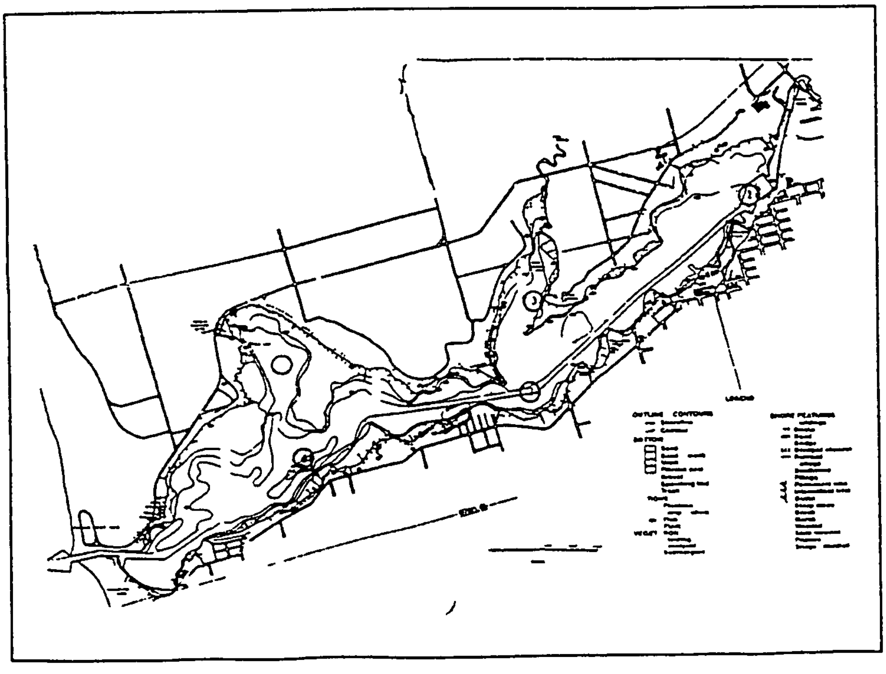
Receiving Water Quality Calibration Examples

十七、總量管制應用實例說明

密西根 Macatawa 湖特性，總湖面積為 1,780 英畝集水區面積 114,560 英畝，平均水深 12 英呎，最大水深 40 英呎，資料顯示此湖有優養化狀態，有高的磷含量及高的葉綠素 a，較高濁度、低溶氧及高的沉澱物，有 44 個點源污染水源區，非點源污染佔 91%總磷之比例。

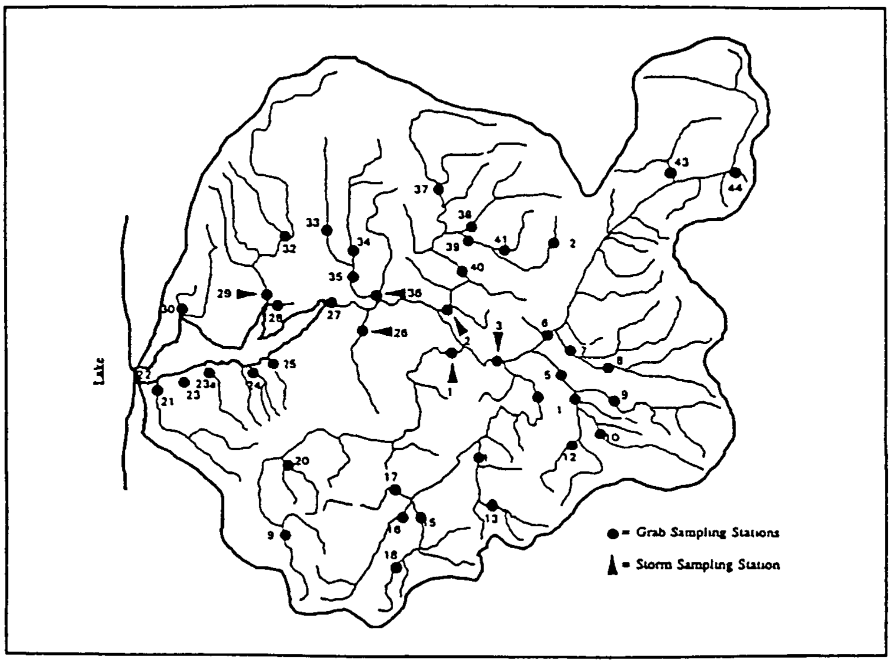
取樣分別在 84 年、85 年及 86 年，分 5 站，取樣分表面、底層及中間深度，共分總磷、硝酸鹽、亞硝酸鹽、氨、懸浮微粒、總溶解固體、葉綠素 a 為整個深度皆量測另在 5 英呎深度增加監測透明度、溫度、溶氧、電導度及酸鹼質，流域圖如 34。

圖 34　密西根 Macatawa 流域圖



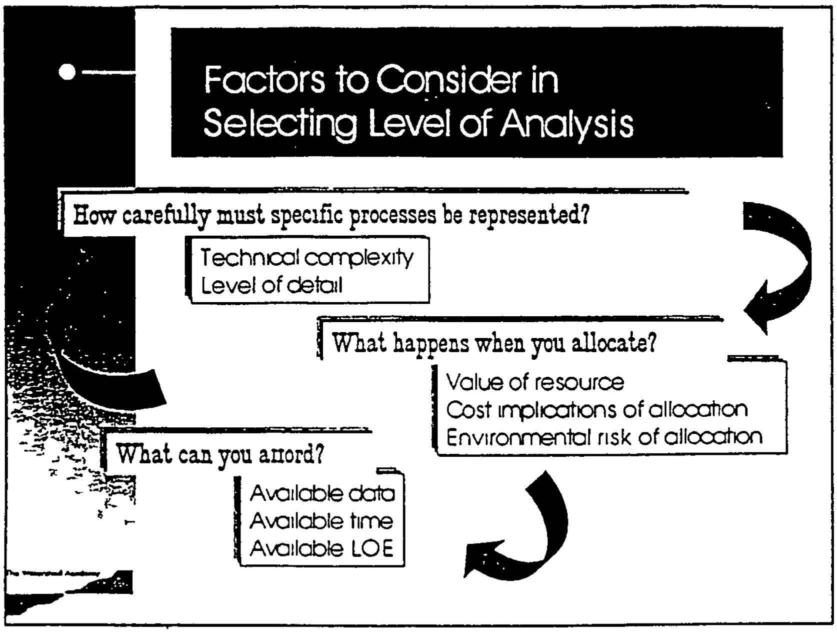
指定用途為水生動物生活及遊憩，整治目標為達到 0 5mg/L 總磷標準，集水區測站共 44 站每月 2 次，6 個自動雨季測站，使用 USGS 儀器每天測流量，測站分佈圖如 35。

圖 35　密西根 Macatawa 流域總量管制測站位置圖



建立總量管制從模式考慮有選擇 BATHTVB, GWIF, AGNPs, SWAT, SWMM, HSPF，從中選擇最適模式為 HSPF，而考慮選擇分析程度時如污染負荷分配必須斟酌污染源價值，總量分配、經費及可交換性，總量分配時對環境危害影響，必須考慮本身可承受之因子如可利用數據，可利用時間等等詳如圖 36。

圖 36　總量分析時考慮因素



Factors to Consider in Selecting Level of Analysis

How carefully must specific processes be represented?

Technical complexity
Level of detail

What happens when you allocate?

Value of resource
Cost implications of allocation
Environmental risk of allocation

What can you afford?

Available data
Available time
Available LOE

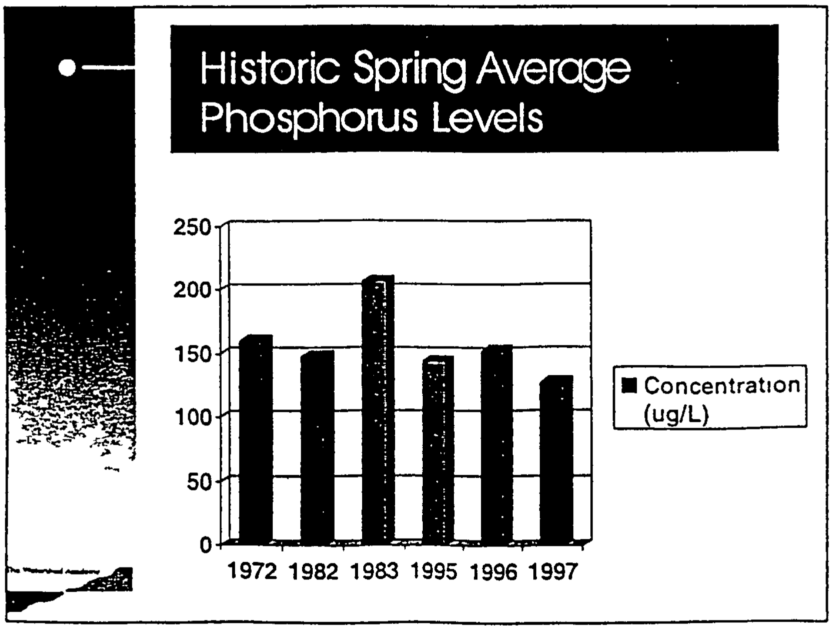
模式考量所需資料為水庫進口之磷濃度，根據以下基礎，所得水庫歷史平均磷濃度如圖 37。

1 每年磷負荷

2 水利停留時間

3 平均水庫深度

圖 37　水庫歷史平均磷濃度



Historic Spring Average Phosphorus Levels

模式不確定因素如下

1 密西根水庫入侵

2 密西根水庫熱邊際效應

3 大的流量導致磷繞流

4 上游濕地可能移掉總磷

污染負荷在此案，可分為非點源污染及點源水污染，非點源污染估計方式如下

1 評估每天負荷

2 根據化學偵測及6個自動測站監測

3 找尋最適分層

4 估計79%排放面積

另未評估到排放面積以平均年負荷來外插，經評估結果，總負荷約126,100lbs。點污染源估計方式主要從44個點源而得，估計每年負荷為12,418 lbs，目前可允許負荷量為33,839 lbs/year，而在夏季點源佔總污染量具較高比率。

經模式評估本案總量分配如下

1 總量管制分配污染負荷量為55,000 lbs/year

2 點源分配污染負荷量為20,000 lbs/year

3 非點源分配污染負荷量為35,000 lbs/year

此項負荷量包括72%在非點源之削減及自然背景上

4 安全係數並不直接故未考慮

本總量管制之完成階段根據模式評估預計以非點源最佳管理計畫(BMPS)可減少 75％污染負荷，另富地地方策略及計畫須由地方政府來完成。

再確認計畫如下

1 預計於西元 2008 年再確認

2 評估是否已達水體水質標準

3 0 50mg/l 總磷濃度為目標

4 較早再確認為達以下標準

(1)每年負荷減少 90,000 lbs/year

(2)磷濃度達到水體水質標準

十八、總量管制模式應用實例

➢實例 1

(1)美國馬里蘭州 Lower Beaverdam Creek 集水區

以下案例應用 BAINS 於美國馬里蘭州的 Lower Beaverdam Creek 集水區，於 BAINS 整合土地利用、河川、氣象、水質等資料，並利用 NPSM 非點源污染模式模擬集水區水質情況進一步推估集水區內污染總量分佈情形。

Lower Beaverdam Creek 集水區面積約 9753acres，主要土地利用型態包括住宅與工業區(74%)、林地(22%)、農業(3%)等，由於集水區內高比例的不透水土地型態，極有可能因雨水逕流造成非源污染。

BASINS 的應用模擬可分為三個階段，分別為資料蒐集彙整、模式校驗、及結果輸出。BASINS 模擬需使用土地利用、河川、集水區邊界等 GIS 資料，Lower Beaverdam Creek 集水區 GIS 如圖 38(土地利用)及圖 39(集水區範圍)所示，圖中 Lower Beaverdam Creek 集水區被細分為 25 個子集水區，子集水區劃分可利用 BASINS Watershed Delineation Tool 依數值高程資料完成。另外，當地氣象資料亦經由 BASINS 氣象檔編寫工具製作為氣象檔，以模擬連續時間之水質變化。

此案例以、BASINS 中 NPSM 非點源污染模式進行模擬，NPSM 可根據降雨、溫度、土地利用型態、和土壤特性作為基本輸入資料，模擬水量、水質隨時間變化情形。首先以實測流量

資料，包括集水區出流點流量、高-低流量分佈型式、暴雨流量、流量季節變化等資料進行水文參數率定，率定結果如圖 40 至圖 41 所示。水文模擬完成後，再以實測水質資料進行水質模擬及水質參數率定，模擬項目包括 BOD、總磷、總氮及鋅、鉛等重金屬，模擬污染物濃度隨時間之變化情形結果如圖 42 至圖 44 所示。

根據水質模擬結果，BASINS 可進一步配合各子集水區土地利用型態及面積估算各子集水區年污染輸出量，如圖 45 至圖 49 所示，由此即可分析 Lower Beaverdam Creek 集水區年單位面積污染負荷量，為 decision-maker 提供集水區規劃管理必要之資訊。

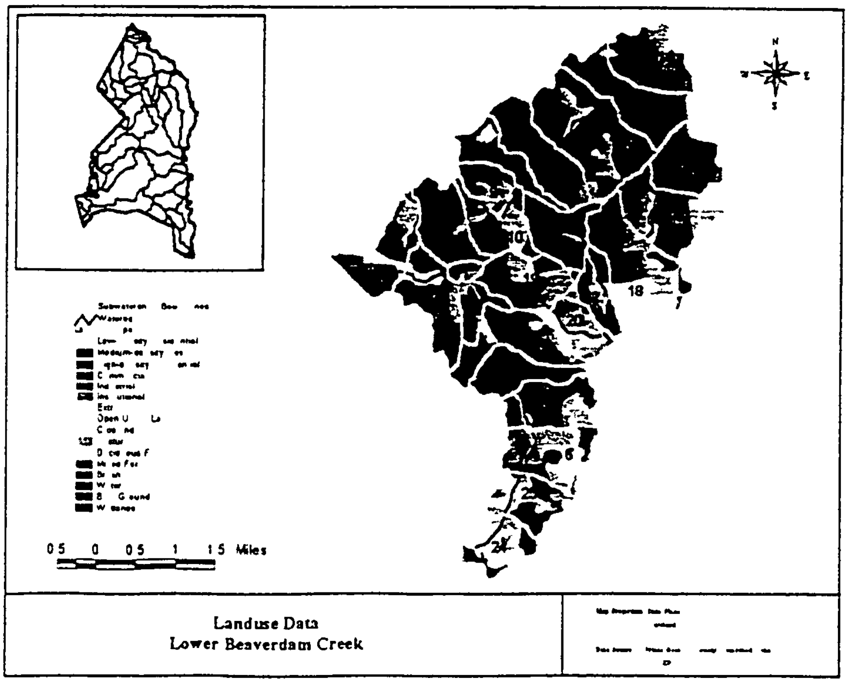


圖 38 Lower Beaverdam Creek 集水區土地利用

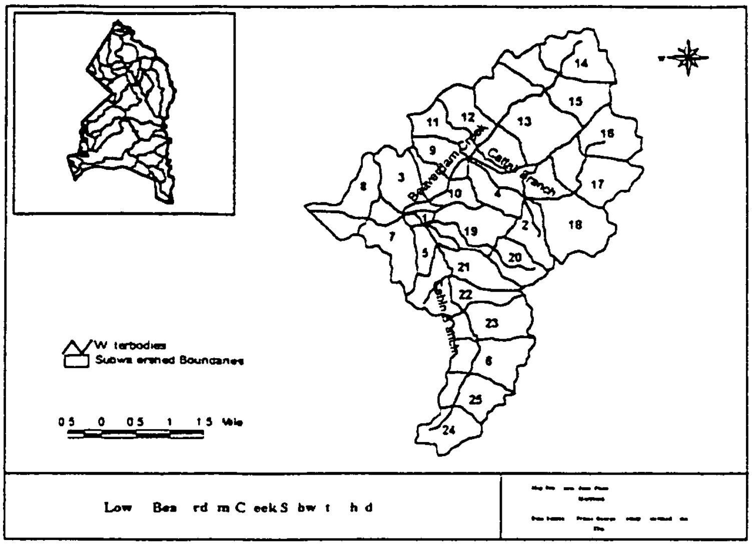


圖 39 Lower Beaverdam Creek 集水區

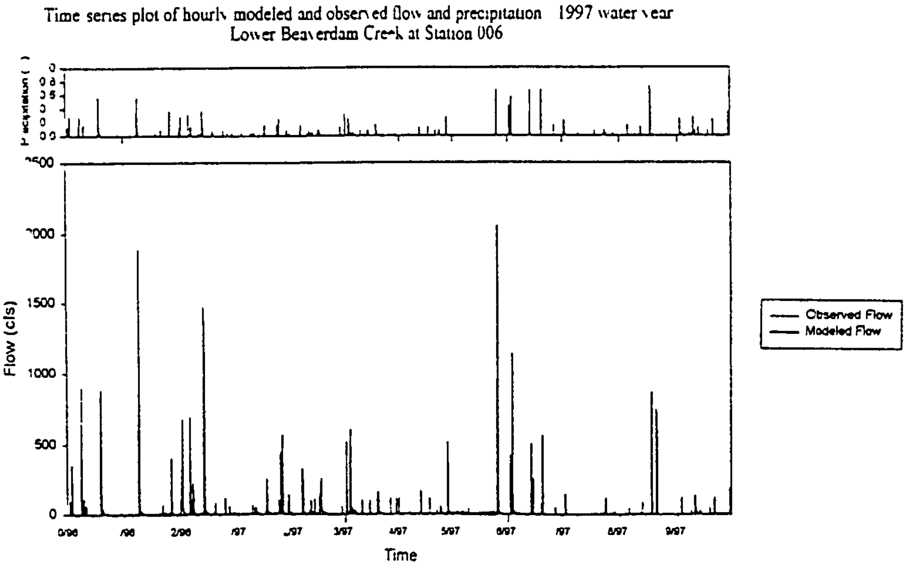


圖 40 水文模擬率定结果

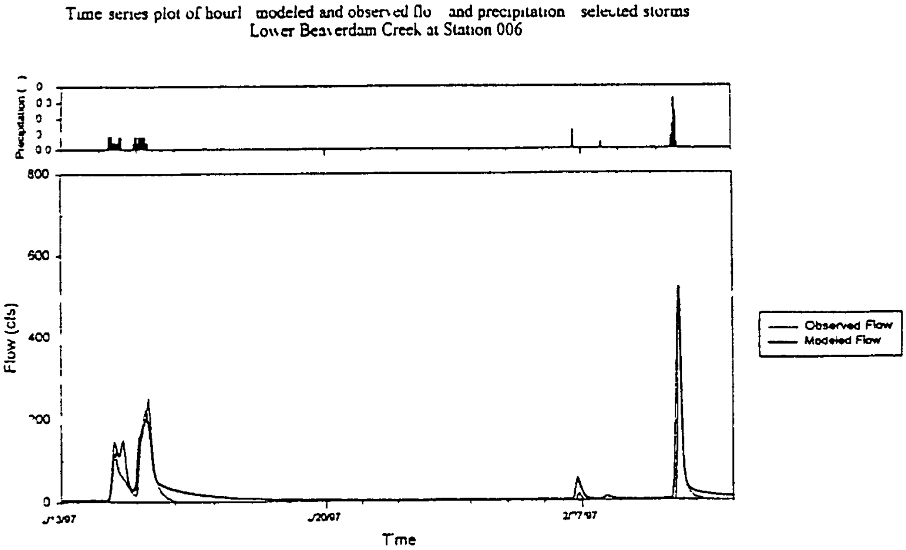
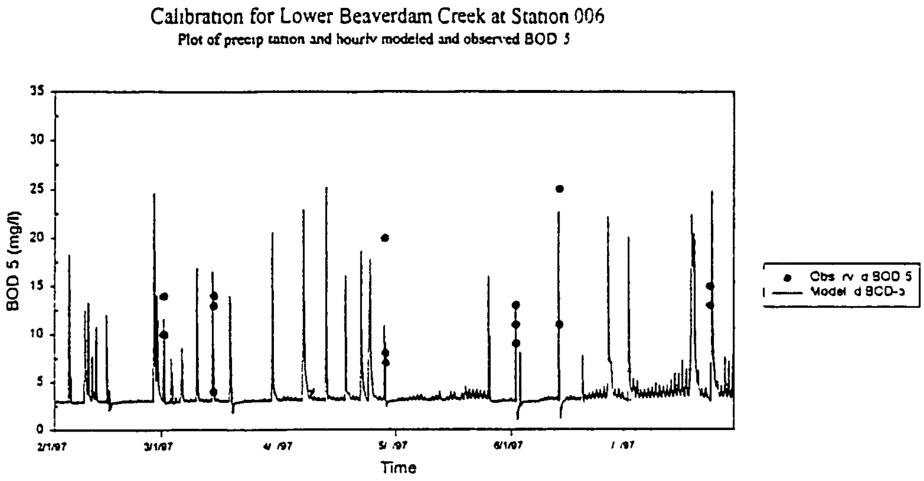


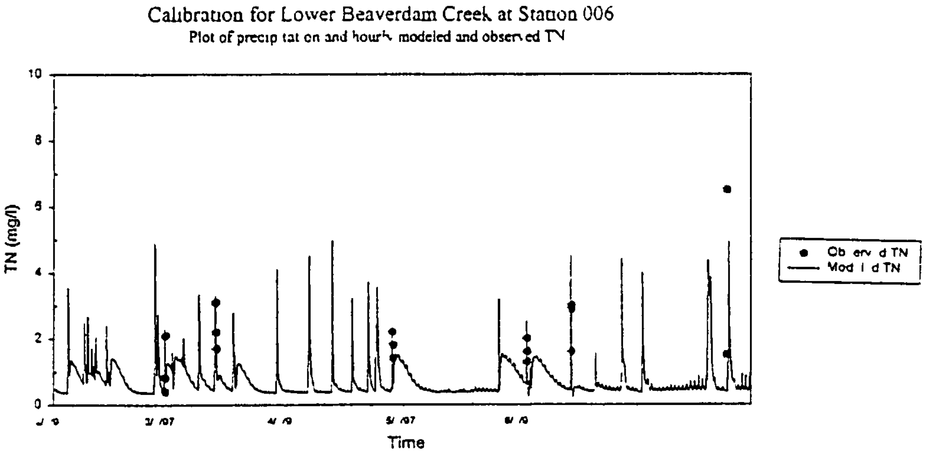
圖 41 單場暴雨模擬率定结果



Calibration for Lower Beaverdam Creek at Station 006

Plot of precipitation and hourly modeled and observed BOD 5

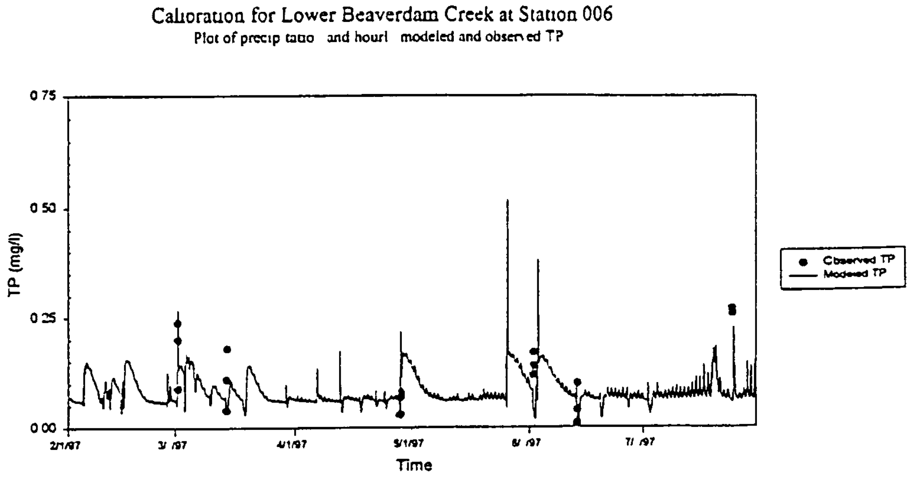
圖 42 BOD模擬率定结果



Calibration for Lower Beaverdam Creek at Station 006

Plot of precipitation and hourly modeled and observed TN

圖 43 總氮模擬率定结果



Calibration for Lower Beaverdam Creek at Station 006

Plot of precipitation and hourly modeled and observed TP

圖 44 總磷模擬率定结果

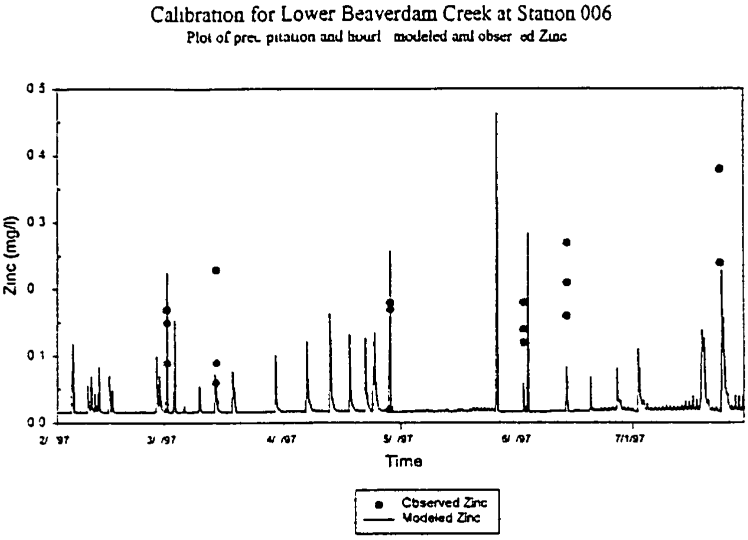


圖 45　鋅模擬率定结果

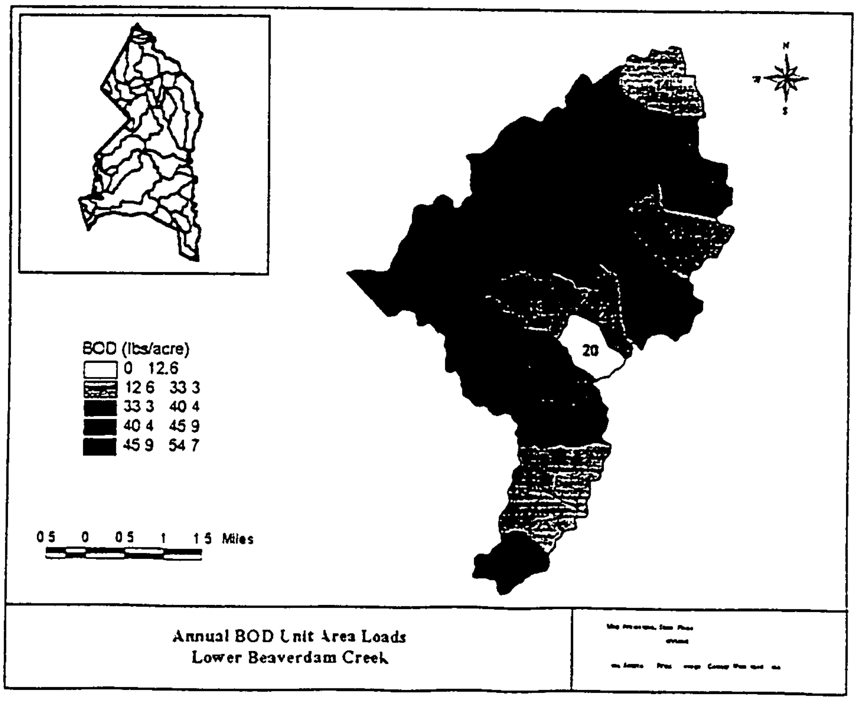


圖 46　BOD 年單位輸出量

圖 47　總氮年單位輸出量

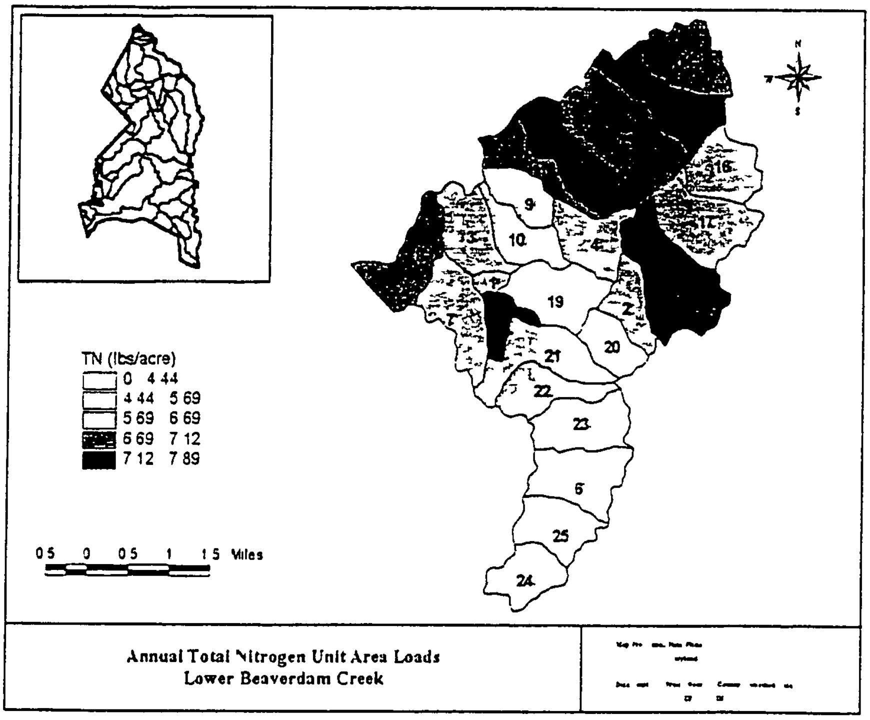


圖 48　總磷年單位輸出量

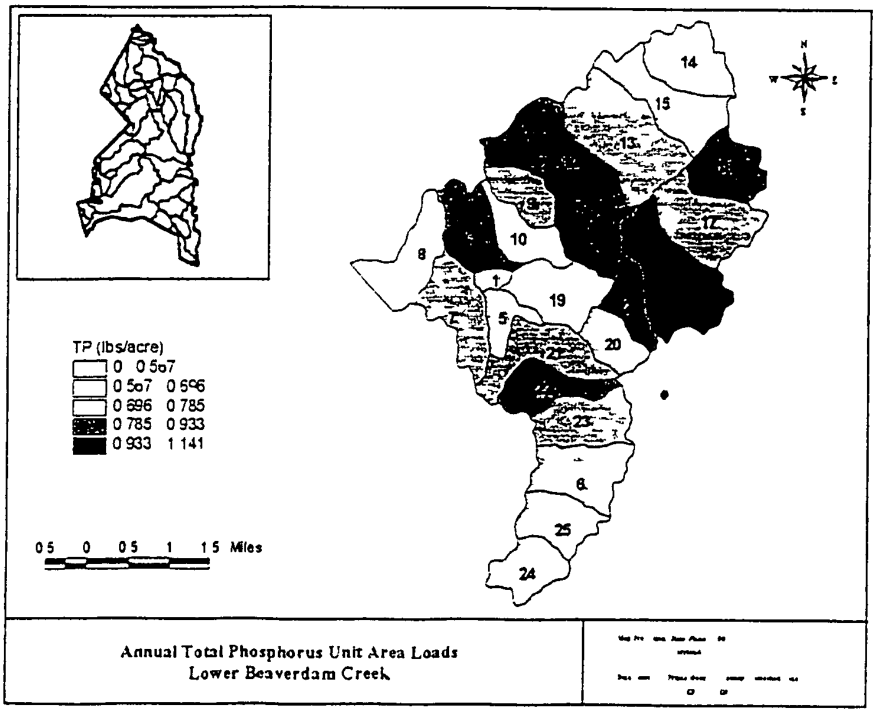
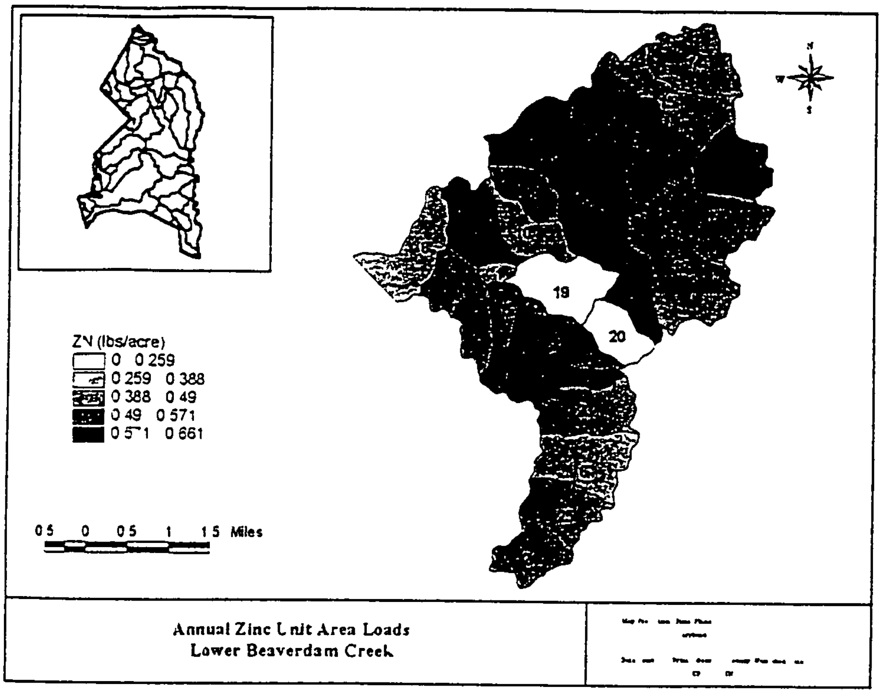


圖 49　鋅年單位輸出量



➢實例 2

Wright, *et al* (1998)利用 QUAL2E 模式模擬美國 Blackstone River(如圖 50 所示)，Blackstone River 長 0 2miles，在計算上將其分 25 個 reaches, 229 個 elements。模擬的項目有 Flow $CBOD_5$, TKN, Ammonium NO_2+NO_3 Ortho-P Chl-a 及 DO 等，模式與實測結果如圖 51 所示，結果顯示吻合度良好。

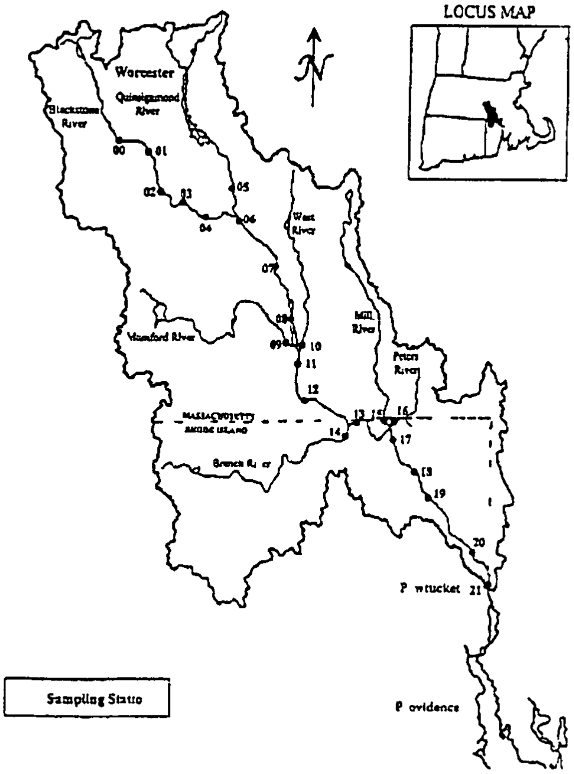


圖 50　Blackstone River 及其集水區示意圖

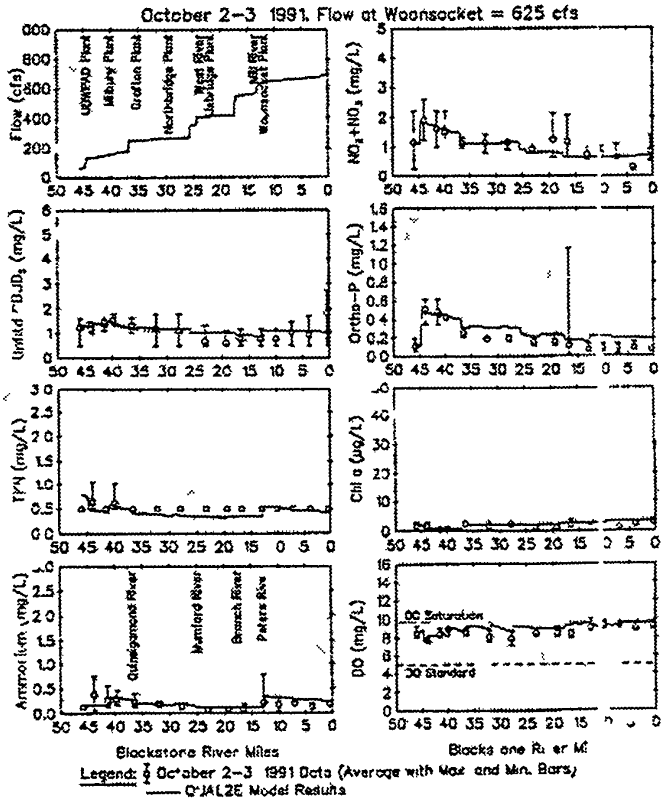


圖 51　模擬與實測結果

➢實例 3

Lung and Larson (1995)利用 WASP5 模式模擬美國 Upper Mississppi River and Lake Pepin (如圖 52 所示)，從 Lock & Dam No 1 到 Lock & Dam No 2 分割成 81 分段(segment)，從 Lock & Dam No 2 到 lake 的出口分割成 80 分段，每個分段長約 4 公尺。圖 53 為 Total P 模擬與實測結果。

194 USING THE WASP AND EUTRO MODELS

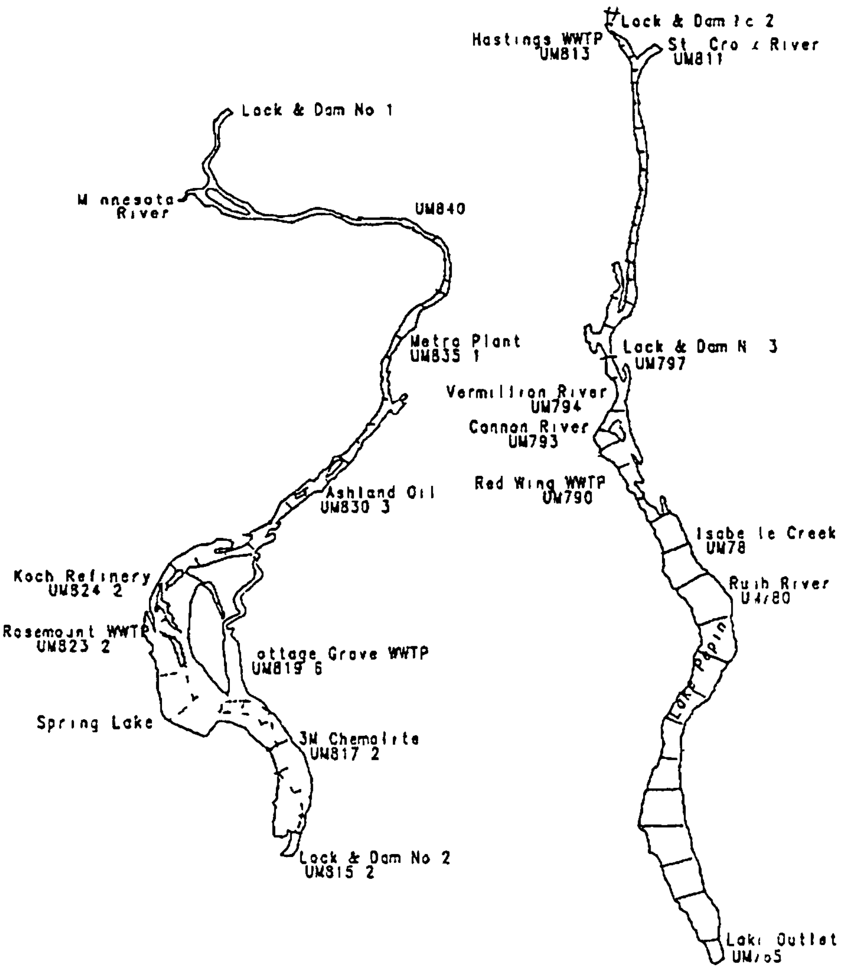


圖 52 Upper Mississppi River and Lake Pepin 示意圖

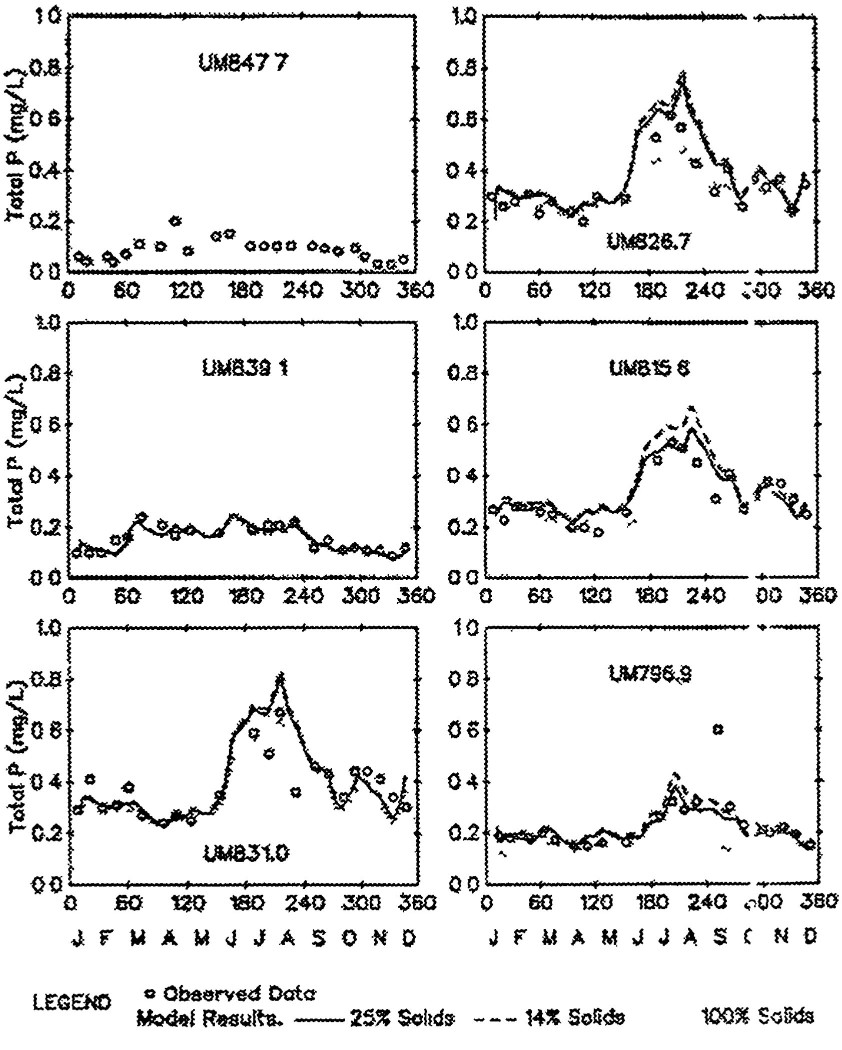


圖 53 Total P 模擬與實測结果

參、心得與建議

一、由於全國河川中高屏溪點源與非點源資料庫較為齊全，建議可以高屏溪為優先進行示範性總量管制之措施。

二、以各種不同模式進行不同河川測試以選擇較適當之適合模式。

三、發展非點源模式，且配合非點源加強宣導，目前管制非點源之營建工地、工業已強制執行，未來可擴展到農業、社區及遊憩等不同之非點源污染防治發展。

四、點源已有許多成熟模式，然需配合總量分配，以達成功效，另下水道應需加強進行，方能使未來總量管制進行順利。

五、發展完善水質監測計畫以提供總量管制模式之校正、驗證及審定。

六、總量管制項目以目前模式可輸出項目如 BOD、NH3-N 及 T-P 為未來總量管制之主要項目。

七、美國總量管制步驟已從有機物如 Nitrogen、phosphate、COD、BOD，發展到以人造有機物 PCB 和重金屬如 Hg，故模式應繼續修正，台灣目前尚未有總量管制方式，應加速腳步，急起直追，以使總量管制模式落實在水污染管制中，使水質更加清澈。

八、國內目前僅使用單一模式且多為河川或水庫數學模式，為考慮水質集水區及承受水體三者合一再加上總量分配為一總合

總量模式，此乃台灣水污染管制當務之急。

九、模式校正及驗證都需大量監測資料，目前台灣所有較齊全資料多集中於水質數據，對於集水區 GIS 資料尚缺乏，故應盡速建立集水區資料以達模式在總量管制之應用。

十、台灣應立即著手作總量管制(相差美國有 20 年以上)初步工作，包括加強立法、總量管制制度宣導、建立，集水區資料建立以逐項趕上先進國家(如美國)水污染管制工作。

十一、模式一般都相當複雜，在模式建立時應建立一套民眾參予總量管制模式應用之機制，以使在總量管制工作上，所受阻力較少，讓民眾對總量管制模式一同參予，以增加總量管制之支持度及接受度。

十二、國內應發展整合模式如 BASINS〔FSPA+QUALE+MODULE(削減模組)〕及 Warmf 模式以整合點源及集水區非點源污染進而以一 MODULE(模組)進行污染負荷削減，運用在總量管制上，如僅發展點源或非點源水污染模式，此方向是質疑且較為不適用的。

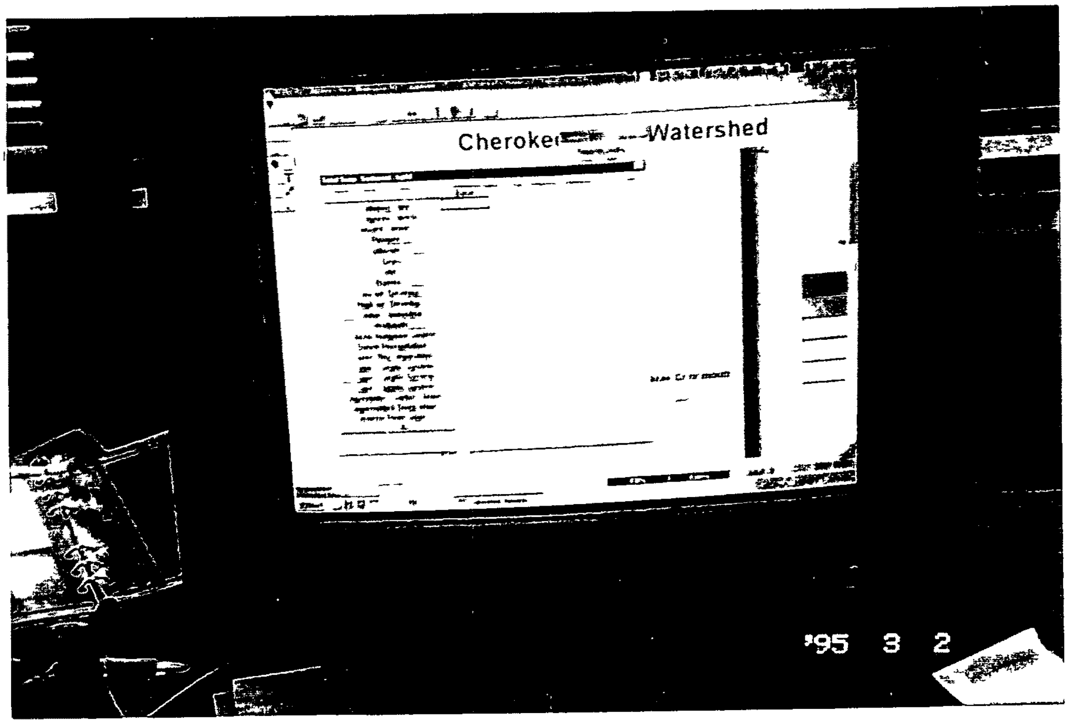
十三、點污染之總量管制在下水道系統尚未建立及國內自動監測系統尚未成熟時，實施上較先進國家困難，如何在此困境下訂定一個適當地總量管制策略是決策者與研究者的一大挑戰。若以近期之可能發展情形而言，初期宜以事業廢水為進行總量管制之主要對象，在監測系統未建立前，可配合排放

許可制度及徵收排放費進行總量管制。

十四、在進行非點源污染分析時，往往需要借重數學模式協助行，然而目前並沒有通用的本土化非點源模式，雖然美國有相當多的模式或估算程序，但因國內特性坡度、土壤特性雨量強度、污染特性均與國外不甚相同，應用於國內情形時會有估計量達數倍誤差之結果，有必要探討各模式之適性，進一步將其本土化。並配合不同工作需要，分別發展確度、難易程度、複雜程度不同之模式，尤其是國內基本料不全，故應加強資料收集、建立及完整性，以發展一個當模式，應用於總量管制非點源模式之分析工作。

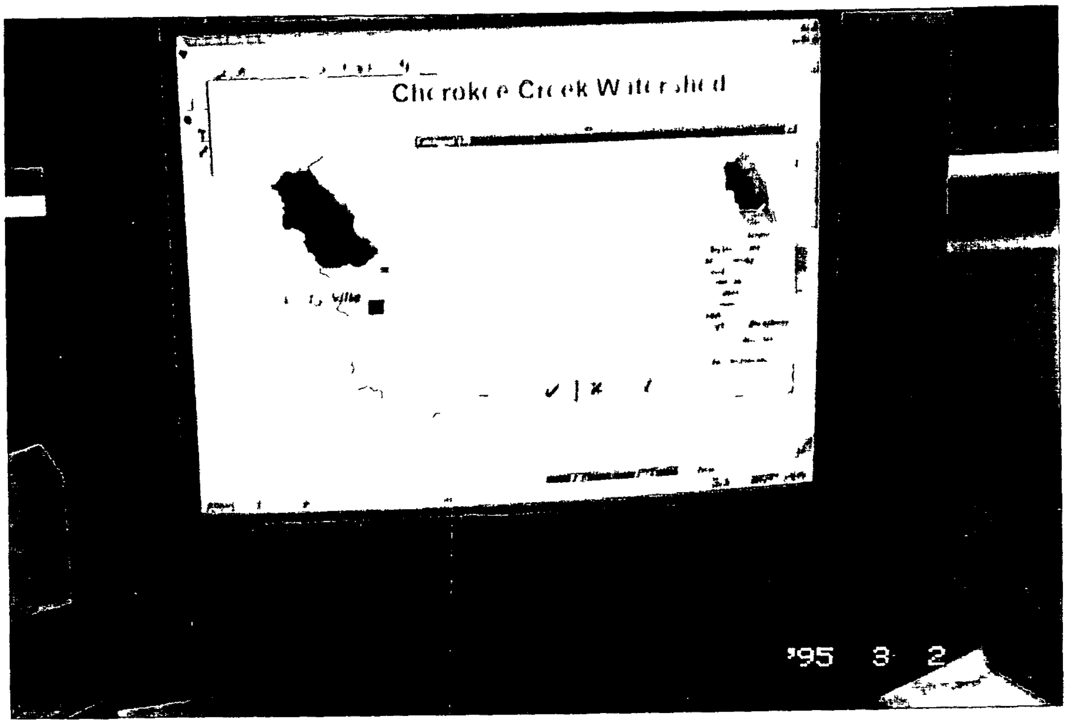
總量管制模式應用參訪

總量管制模式應用參訪

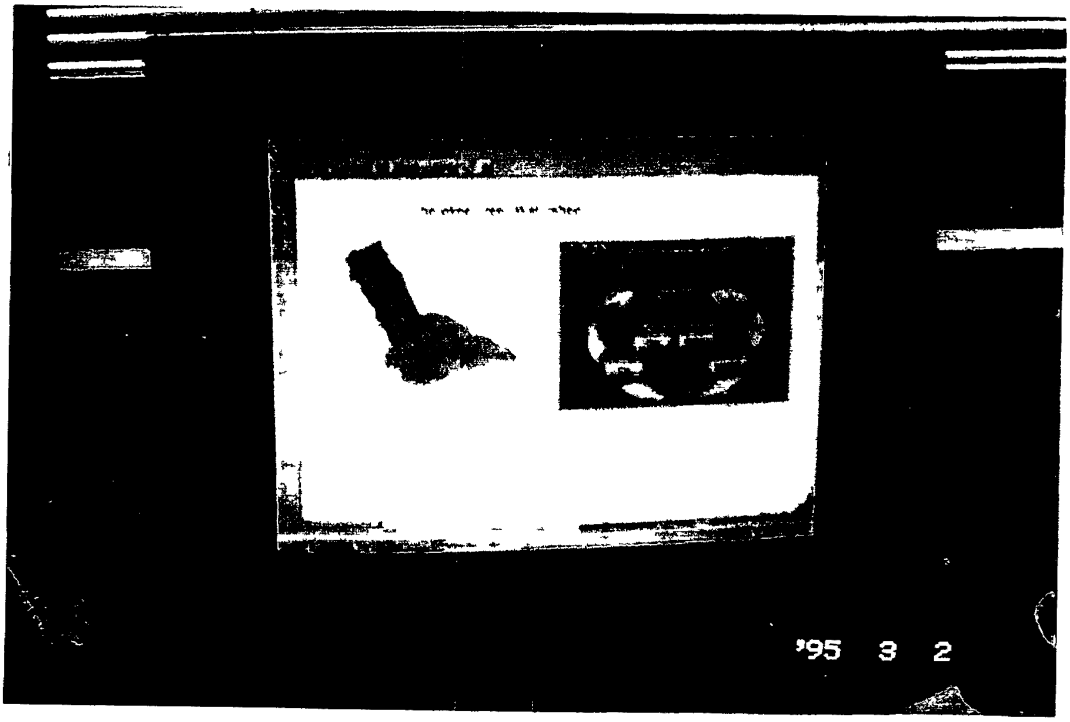


總量管制模式應用實際電腦操作

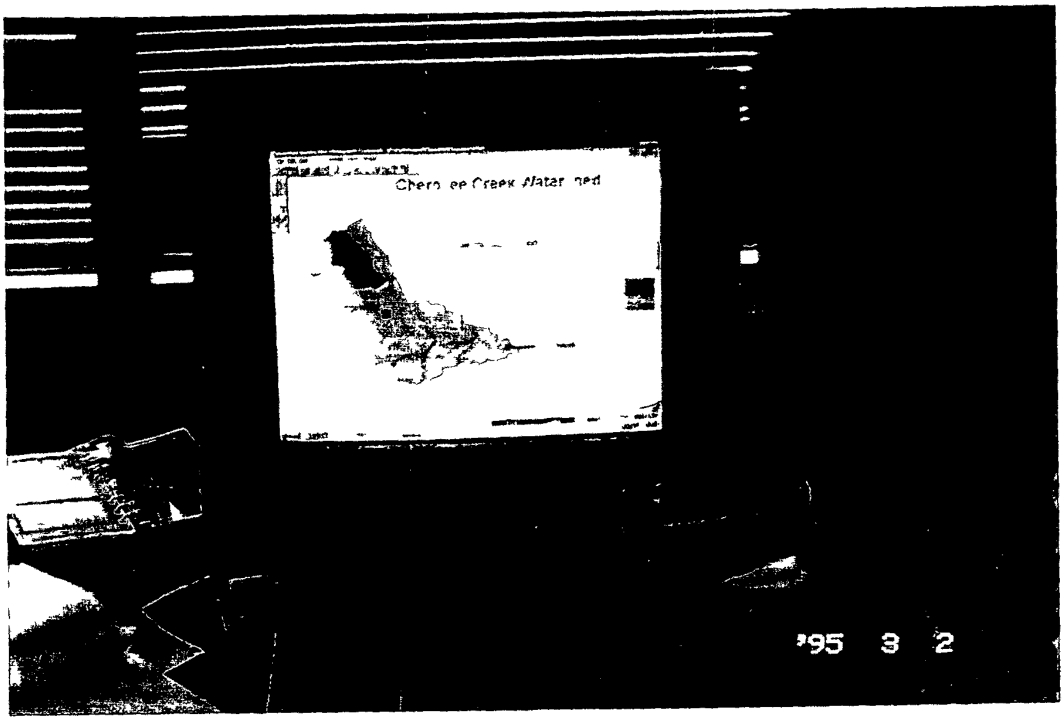
總量管制模式應用實際電腦操作



總量管制模式應用實際電腦操作



總量管制模式應用實際電腦操作



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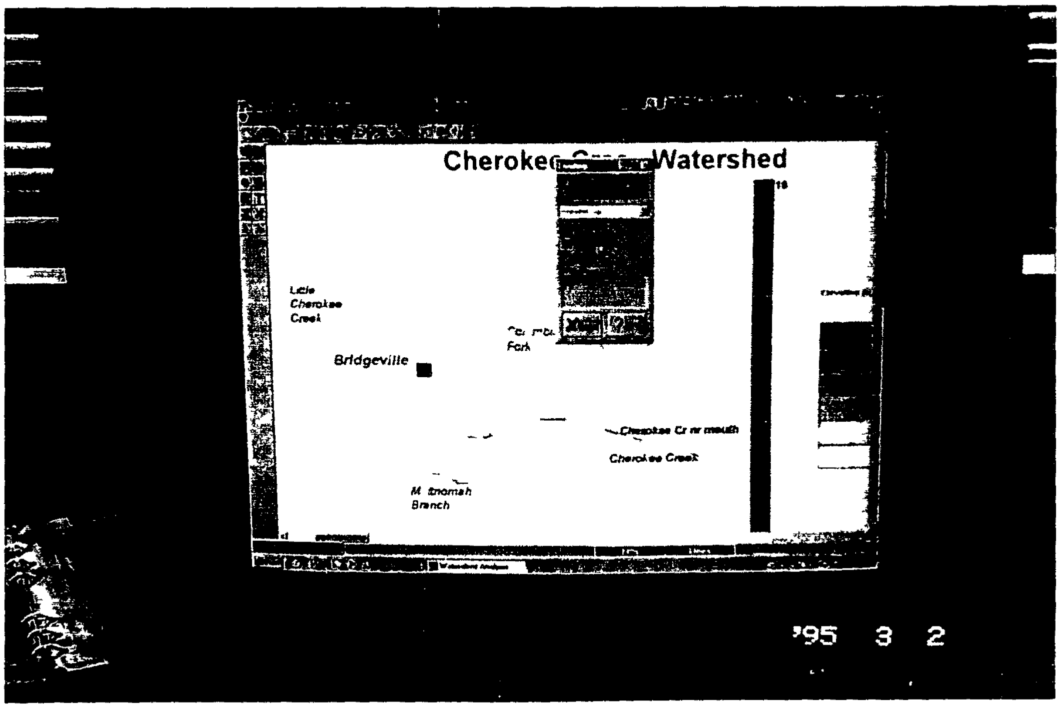

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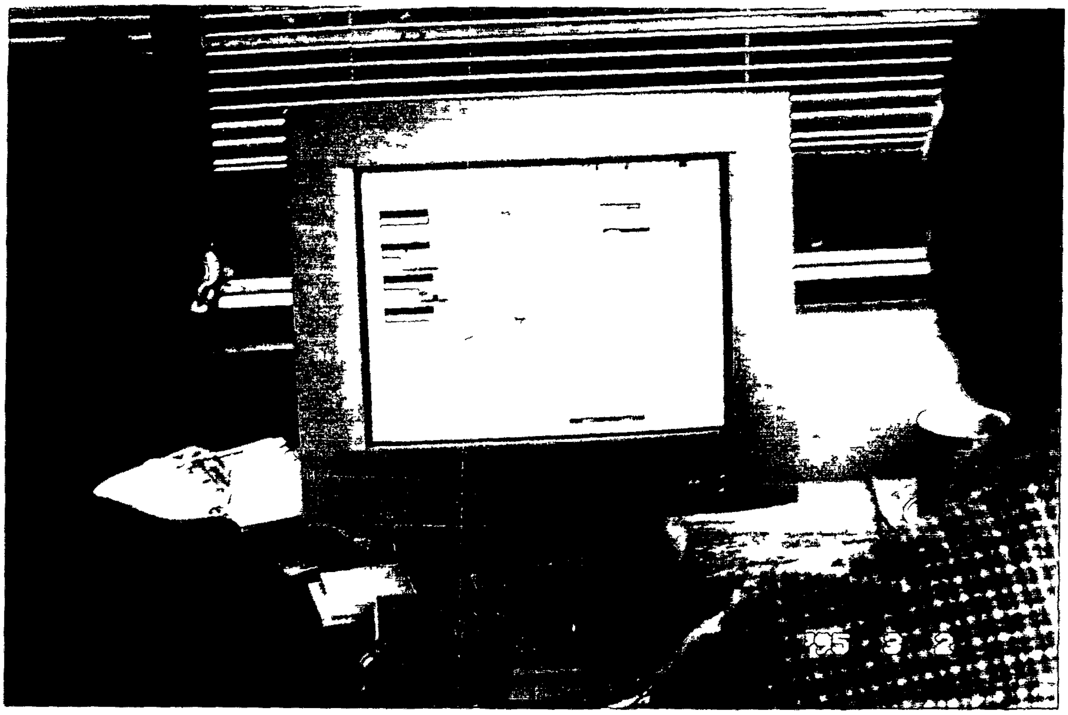

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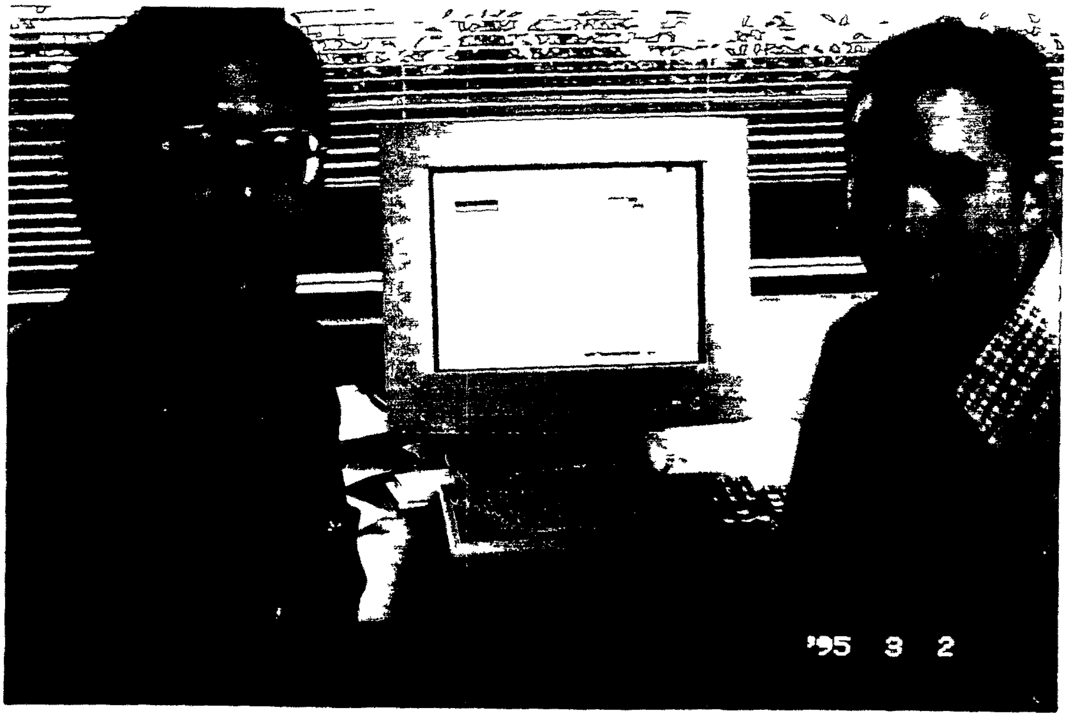

總量管制模式應用實際電腦操作

肆、附錄

(一)The Water quality analysis simulation program wasps ASCI corporation Athens, Georgia 30605

(二) The Enhanced stream water quality model Qual2e and Qual2e-UNCAS, Environmental research laboratory Athens, GA 30613

附錄　一

June 25, 1993

THE WATER QUALITY ANALYSIS SIMULATION PROGRAM, WASP5

PART A:

MODEL DOCUMENTATION

by

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CONTENTS

FIGURES

TABLES

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CHAPTER 1

INTRODUCTION TO THE WASP5 MODEL

The Water Quality Analysis Simulation Program--5 (WASP5), an enhancement of the original WASP (Di Toro et al , 1983) helps users interpret and predict water quality responses to natural phenomena and man-made pollution for various pollution management decisions WASP5 is a dynamic compartment modeling program for aquatic systems including both the water column and the underlying benthos. The time-varying processes of advection, dispersion, point and diffuse mass loading, and boundary exchange are represented in the basic program

Water quality processes are represented in special kinetic subroutines that are either chosen from a library or written by the user WASP is structured to permit easy substitution of kinetic subroutines into the overall package to form problem-specific models WASP5 comes with two such models -- TOXI5 for toxicants and EUTRO5 for conventional water quality Earlier versions of WASP have been used to examine eutrophication and PCB pollution of the Great Lakes (Thomann, 1975, Thomann et al , 1976, Thomann et al, 1979, Di Toro and Connolly, 1980). eutrophication of the Potomac Estuary (Thomann and Fitzpatrick, 1982) kepone pollution of the James River Estuary (O'Connor et al , 1983) volatile organic pollution of the Delaware Estuary (Ambrose, 1987), and heavy metal pollution of the Deep River, North Carolina (JRB 1984) In addition to these, numerous applications are listed in Di Toro et al , 1983

EUTRO5

The flexibility afforded by the Water Quality Analysis Simulation Program is unique WASP5 permits the modeler to structure one, two and three dimensional models, allows the specification of time-variable exchange coefficients, advective flows, waste loads and water quality boundary conditions and permits tailored structuring of the kinetic processes, all within the larger modeling framework without having to write or rewrite large sections of computer code The two operational WASP5 models, TOXI5 and EUTRO5, are reasonably general In addition, users may develop new kinetic or reactive structures This, however requires an additional measure of judgment insight and programming experience on the part of the modeler The kinetic subroutine in WASP (denoted WASPB"), is kept as a separate section of code, with its own subroutines if desired

1 1 OVERVIEW OF THE WASP5 MODELING SYSTEM

The WASP5 system consists of two stand-alone computer programs, DYNHYD5 and WASP5, that can be run in conjunction or separately (Figure 1 1) The hydrodynamics program, DYNHYD5, simulates the movement of water while the water quality program, WASP5, simulates the movement and interaction of pollutants within the water While DYNHYD5 is delivered with WASP5, other hydrodynamic programs have also been linked with WASP RIVMOD (Hosseinipour, 1990) handles unsteady flow in one-dimensional rivers, while HYDRO3D handles unsteady, three-dimensional flow in lakes and estuaries

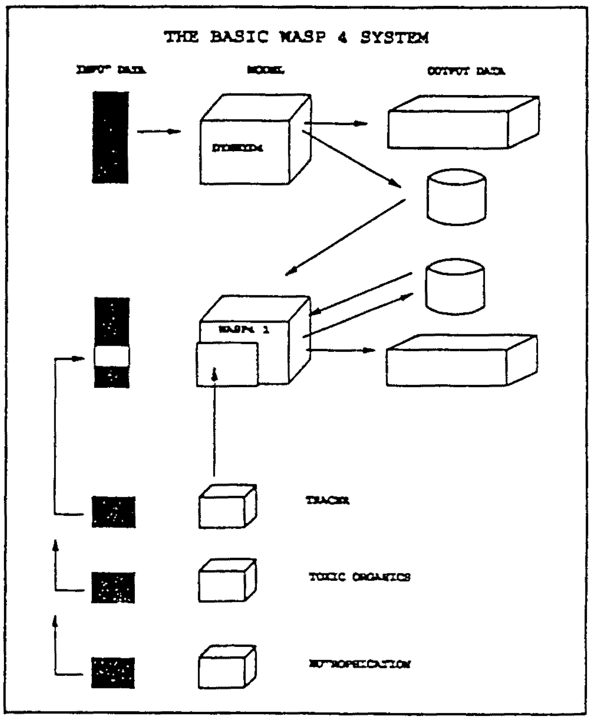


Figure 1 1 The basic WASP5 system

WASP5 is supplied with two kinetic sub-models to simulate two of the major classes of water quality problems conventional pollution (involving dissolved oxygen biochemical oxygen demand nutrients and eutrophication) and toxic pollution (involving organic chemicals, metals and sediment) The linkage of either sub-model with the WASP5 program gives the models EUTRO5 and TOXI5 respectively This is illustrated in Figure 1 1 with blocks to be substituted into the incomplete WASP5 model The tracer block can be a dummy sub-model for substances with no kinetic interactions In most instances, TOXI5 is used for tracers by specifying no decay

The basic principle of both the hydrodynamics and water-quality program is the conservation of mass The water volume and water-quality constituent masses being studied are tracked and accounted for over time and space using a series of mass balancing equations The hydrodynamics program also conserves momentum, or energy, throughout time and space

1 2 THE BASIC WATER QUALITY MODEL

WASP5 is a dynamic compartment model that can be used to analyze a variety of water quality problems in such diverse water bodies as ponds streams, lakes, reservoirs, rivers estuaries, and coastal waters This section presents an overview of the basic water quality model Subsequent chapters detail the transport and transformation processes in WASP5 for various water quality constituents

The equations solved by WASP5 are based on the key principle of the conservation of mass This principle requires that the mass of each water quality constituent being investigated must be accounted for in one way or another WASP5 traces each water quality constituent from the point of spatial and temporal input to its final point of export, conserving mass in space and time To perform these mass balance computations, the user must supply WASP5 with input data defining seven important characteristics

simulation and output control
model segmentation
advective and dispersive transport
boundary concentrations
point and diffuse source waste loads
kinetic parameters, constants, and time functions
initial concentrations

These input data, together with the general WASP5 mass balance equations and the specific chemical kinetics equations, uniquely define a special set of water quality equations These are numerically integrated by WASP5 as the simulation proceeds in time At user-specified print intervals WASP5 saves the values of all display variables for subsequent retrieval by the post-processor programs W4DSPLY and W4PLOT These programs allow the user to interactively produce graphs and tables of variables of all display variables

1 3 THE GENERAL MASS BALANCE EQUATION

A mass balance equation for dissolved constituents in a body of water must account for all the material entering and leaving through direct and diffuse loading advective and dispersive transport and physical chemical and biological transformation Consider the coordinate system shown in Figure 1 2 where the x- and y-coordinates are in the horizontal plane, and the z-coordinate is in the vertical plane The mass balance equation around an infinitesimally small fluid volume is

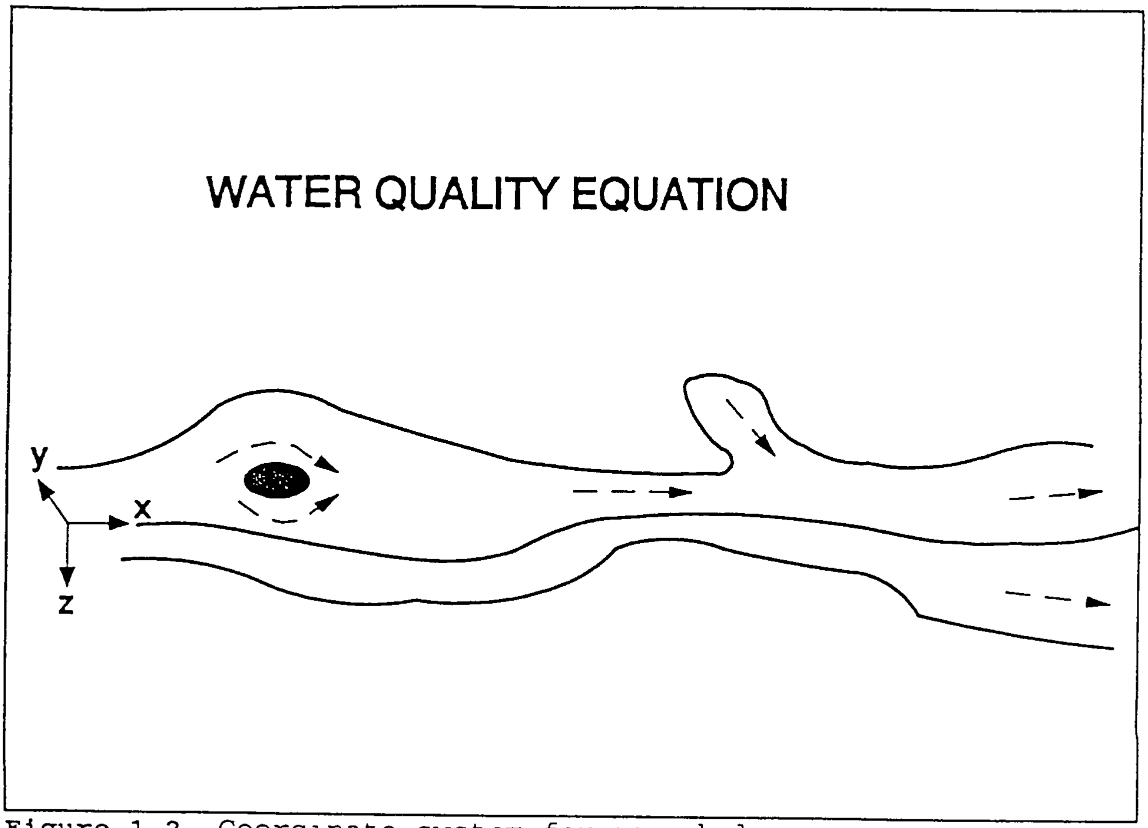


Figure 1 2 Coordinate system for mass balance equation

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(U_x\, C) - \frac{\partial}{\partial y}(U_y\, C) - \frac{\partial}{\partial z}(U_z\, C)$$
$$+ \frac{\partial}{\partial x}(E_x \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(E_y \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z}(E_z \frac{\partial C}{\partial z}) \qquad 1\ 1$$
$$+ S_L + S_B + S_K$$

where

C = concentration of the water quality constituent mg/L or g/m^3

t = time days

U_x, U_y, U_z = longitudinal lateral, and vertical advective velocities m/day

E_x, E_y, E_z = longitudinal, lateral, and vertical diffusion coefficients, m^2/day

S_L = direct and diffuse loading rate g/m^3-day

S_B = boundary loading rate (including upstream downstream benthic, and atmospheric), g/m^3-day

S_K = total kinetic transformation rate, positive is source negative is sink g/m^3-day

By expanding the infinitesimally small control volumes into larger adjoining segments, and by specifying proper transport, loading, and transformation parameters, WASP implements a finite-difference form of equation 1 1 For brevity and clarity however, the derivation of the finite-difference form of the mass balance equation will be for a one-dimensional reach Assuming vertical and lateral homogeneity, we can integrate equation 1 1 over y and z to obtain

$$\frac{\partial}{\partial t}(AC) = \frac{\partial}{\partial x}\left(-U_x AC + E_x A\frac{\partial C}{\partial x}\right) + A\,(S_L + S_B) + AS_K \qquad 1\ 2$$

where

A = cross-sectional area, m^2

This equation represents the three major classes of water quality processes -- transport (term 1), loading (term 2) and transformation (term 3) The finite-difference form is derived in Appendix E The model network and the major processes are discussed in the following sections

1 4 THE MODEL NETWORK

The model network is a set of expanded control volumes or segments that together represent the physical configuration of the water body As Figure 1 3 illustrates, the network may subdivide the water body laterally and vertically as well as longitudinally Benthic segments can be included along with water column segments If the water quality model is being linked to the hydrodynamic model, then water column segments must correspond to the hydrodynamic junctions Concentrations of water quality constituents are calculated within each segment Transport rates of water quality constituents are calculated across the interface of adjoining segments

Segments in WASP may be one of four types, as specified by the input variable ITYPE A value of 1 indicates the epilimnion (surface water), 2 indicates hypolimnion layers (subsurface) 3

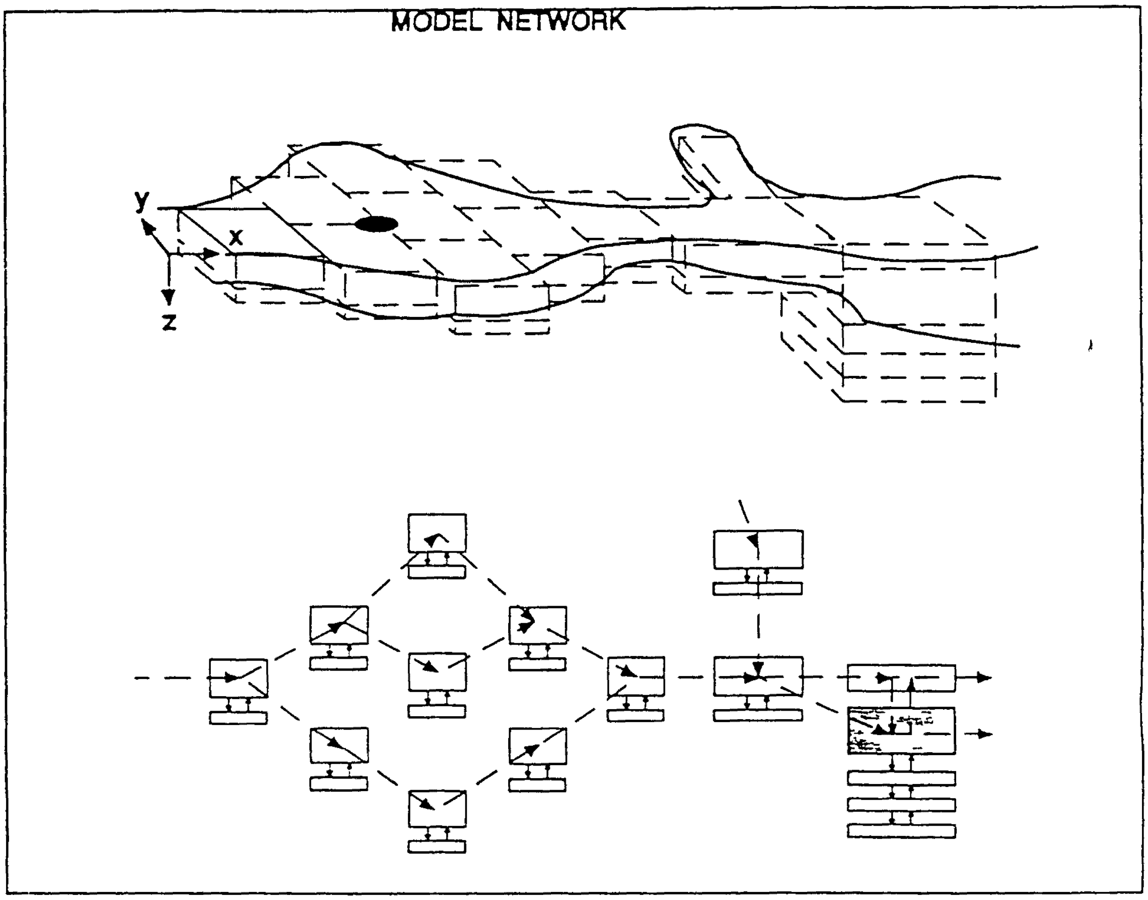


Figure 1 3 Model segmentation

indicates an upper benthic layer, and 4 indicates lower benthic layers The segment type plays an important role in bed sedimentation and in certain transformation processes The user should be careful to align segments properly The segment immediately below each segment is specified by the input variable IBOTSG This alignment is important when light needs to be passed from one segment to the next in the water column or when material is buried or eroded in the bed

Segment volumes and the simulation time step are directly related As one increases or decreases the other must do the same to insure stability and numerical accuracy Segment size can vary dramatically, as illustrated in Figure 1 4 Characteristic sizes are dictated more by the spatial and temporal scale of the problem being analyzed than by the characteristics of the water body or the pollutant per se For example analyzing a problem involving the upstream tidal migration of a pollutant into a water supply might require a time step of minutes to an hour By contrast, analyzing a problem

SPATIAL SCALES USED IN

LAKE ONTARIO ANALYSIS

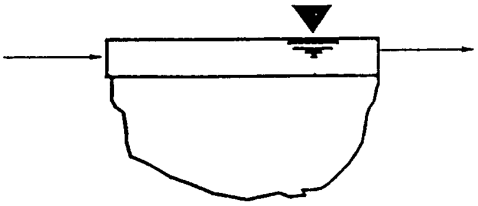
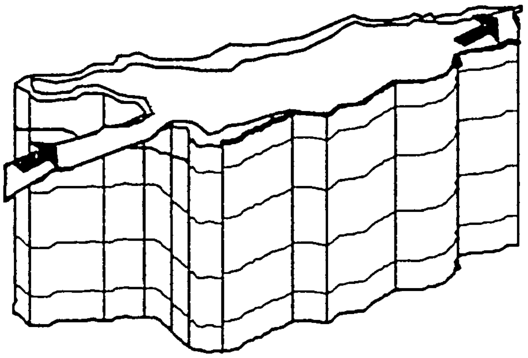
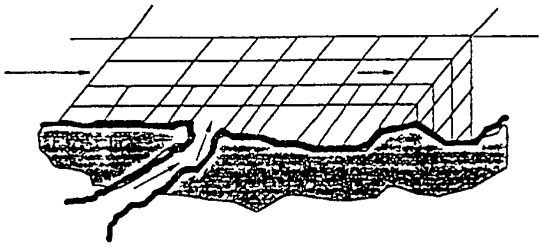
MODEL DESIGNATION		NUMBER OF SEGMENTS	HORIZONTAL SCALE (km) ^{2} EPILIMNION SEGMENTS
LAKE 1		2	13,000
LAKE 3		67	200-1000
ROCHESTER EMBAYMENT		72	10-100

Figure 1 4 Spatial scales used in Lake Ontario analysis good figure

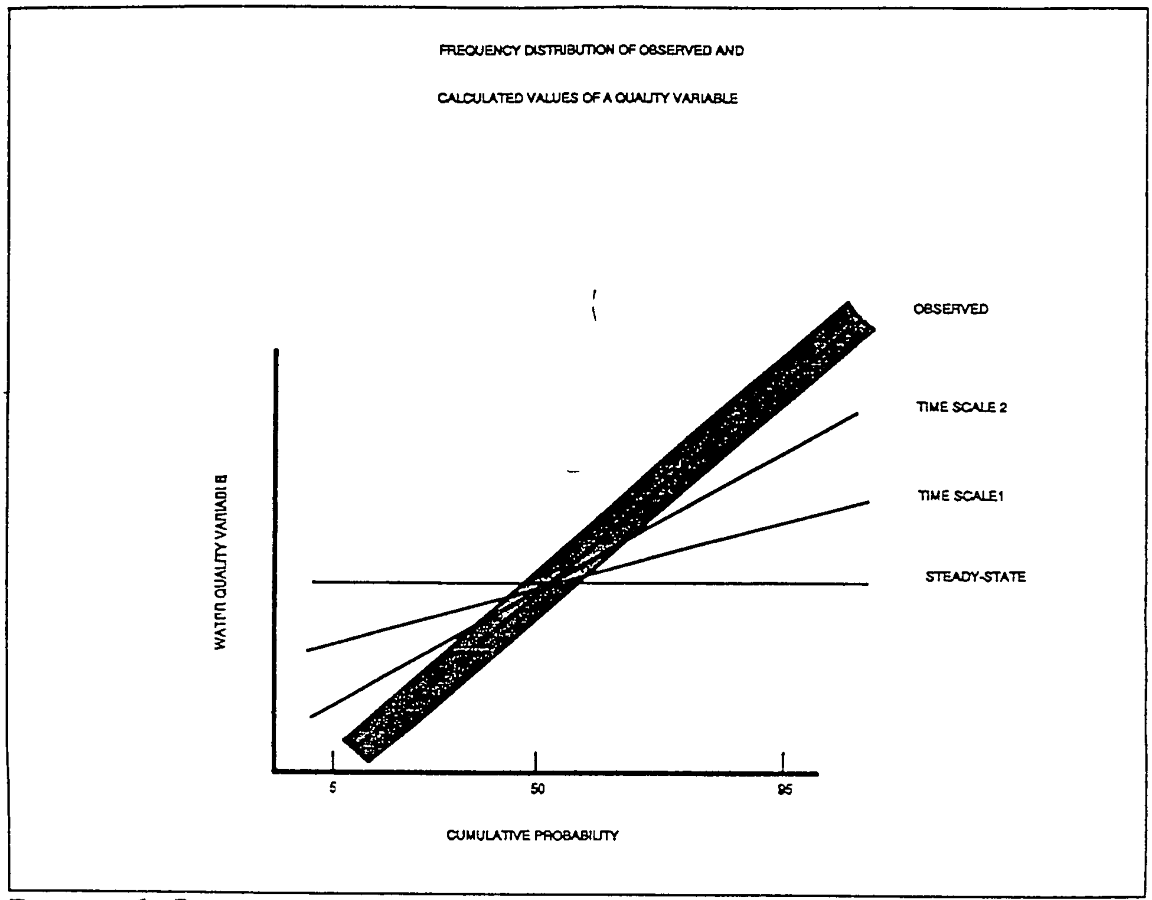


Figure 1 5 Frequency distribution of observed and calculated values of a quality variable

[illegible]

predicted For example, a daily-average dissolved oxygen concentration of 5 mg/L would not sufficiently protect fish if fluctuations result in concentrations less than 2 mg/L for 10% of the time Predicting extreme concentration values is generally more difficult than predicting average values. Figure 1 5 illustrates typical frequency distributions predicted by three model time scales and a typical distribution observed by rather thorough sampling as they would be plotted on probability paper The straight lines imply normal distributions Reducing the model time step (and consequently segment size) allows better simulation of the frequency distribution This increase in predictive ability, however, also entails an increase in the resolution of the input data

[illegible] mixed not and dispersed

Once the nature of the problem has been determined, then the temporal variability of the water body and input loadings must be considered Generally the model time step must be somewhat less than the period of variation of the important driving variables

In some cases, this restriction can be relaxed by averaging the input over its period of variation For example, phytoplankton growth is driven by sunlight, which varies diurnally Most eutrophication models, however, average the light input over a day, allowing time steps on the order of a day

.Care must be taken so that important non-linear interactions do not get averaged out When two or more important driving variables have a similar period of variation, then averaging may not be possible One example is the seasonal variability of light, temperature nutrient input, and transport in lakes subject to eutrophication Another example involves discontinuous batch discharges Such an input into a large lake might safely be averaged over a day or week, because large scale transport variations are relatively infrequent The same batch input into a tidal estuary cannot safely be averaged however because of the semi-diurnal or diurnal tidal variations A third example is salinity intrusion in estuaries Tidal variations in flow, volume, and dispersion can interact so that accurate long-term predictions require explicit simulation at time steps on the order of hours

Once the temporal variability has been determined, then the spatial variability of the water body must be considered Generally, the important spatial characteristics must be homogeneous within a segment In some cases, this restriction can be relaxed by judicious averaging over width depth, and/or length 明智的 For example, depth governs the impact of reaeration and sediment oxygen demand in a column of water Nevertheless, averaging the depth across a river would generally be acceptable in a conventional waste load allocation, whereas averaging the depth across a lake would not generally be acceptable Other important spatial characteristics to consider (depending upon the problem being analyzed) include temperature, light penetration velocity pH benthic characteristics or fluxes and sediment concentrations

The expected spatial variability of the water quality concentrations also affects the segment sizes The user must determine how much averaging of the concentration gradients is acceptable Because water quality conditions change rapidly near a loading point and stabilize downstream studying the effects on a beach a quarter-mile downstream of a discharge requires smaller segments than studying the effects on a beach several miles away

A final, general guideline may be helpful in obtaining accurate simulations water column volumes should be roughly the same why If flows vary significantly downstream then segment volumes should increase proportionately The user should first choose the proper segment volume and time step in the critical reaches of the water body (V_c, Δt_c), then scale upstream and downstream segments accordingly

$$V_i = V_c\, Q_i / Q_c \qquad 1.3$$

Of course, actual volumes specified must be adjusted to best represent the actual spatial variability, as discussed above. This guideline will allow larger time steps and result in greater numerical accuracy over the entire model network, as explained in the section on "Simulation Parameters" in Chapter 2.

1.5 THE MODEL TRANSPORT SCHEME

Transport includes advection and dispersion of water quality constituents. Advection and dispersion in WASP are each divided into six distinct types, or "fields." The first transport field involves advective flow and dispersive mixing in the water column. Advective flow carries water quality constituents "downstream" with the water and accounts for instream dilution. Dispersion causes further mixing and dilution between regions of high concentrations and regions of low concentrations.

The second transport field specifies the movement of pore water in the sediment bed. Dissolved water quality constituents are carried through the bed by pore water flow and are exchanged between the bed and the water column by pore water diffusion.

√ The third, fourth, and fifth transport fields specify the transport of particulate pollutants by the settling, resuspension and sedimentation of solids. Water quality constituents sorbed onto solid particles are transported between the water column and the sediment bed. The three solids fields can be defined by the user as size fractions, such as sand, silt, and clay, or as inorganic, phytoplankton, and organic solids.

The sixth transport field represents evaporation or precipitation from or to surface water segments.

Most transport data, such as flows or settling velocities, must be specified by the user in a WASP input dataset. For water column flow, however, the user may "link" WASP with a hydrodynamics model. If this option is specified during the simulation, WASP will read the contents of a hydrodynamic file for unsteady flows, volumes, depths, and velocities.

1.6 APPLICATION OF THE MODEL

The first step in applying the model is analyzing the problem to be solved. What questions are being asked? How can a simulation model be used to address these questions? A water quality model can do three basic tasks-- ①describe present water quality conditions, ②provide generic predictions, and ③provide site-specific predictions The first, descriptive task is to extend in some way a limited site-specific data base Because monitoring is expensive, data seldom give the spatial and temporal resolution needed to fully characterize a water body A simulation model can be used to interpolate between observed data, locating for example, the dissolved oxygen sag point in a river or the maximum salinity intrusion in an estuary Of course such a model can be used to guide future monitoring efforts Descriptive models also can be used to infer the important processes controlling present water quality This information can be used to guide not only monitoring efforts, but also model development efforts

Providing generic predictions is a second type of modeling task Site-specific data may not be needed if the goal is to predict the types of water bodies at risk from a new chemical A crude set of data may be adequate to screen a list of chemicals for potential risk to a particular water body Generic predictions may sufficiently address the management problem to be solved or they may be a preliminary step in detailed site-specific analyses

Providing site-specific predictions is the most stringent modeling task Calibration to a good set of monitoring data is definitely needed to provide credible predictions Because predictions often attempt to extrapolate beyond the present data base, however, the model also must have sufficient process integrity Examples of this type of application include waste load allocation to protect water quality standards and feasibility analysis for remedial actions, such as tertiary treatment phosphate bans, or agricultural best-management practices

Analysis of the problem should dictate the spatial and temporal scales for the modeling analysis Division of the water body into appropriately sized segments was discussed in Section Model Network The user must try to extend the network upstream and downstream beyond the influence of the waste loads being studied If this is not possible the user should extend the network far enough so that errors in specifying future boundary concentrations do not propogate into the reaches being studied

The user also should consider aligning the network so that sampling stations and points of interest (such as water withdrawals) fall near the center of a segment Point source waste loads in streams and rivers with unidirectional flow should be located near the upper end of a segment In estuaries and other water bodies with oscillating flow, waste loads are best centered within segments If flows are to be input from DYN- D5 then a WASP4 segment must coincide with each hydrodynamic junction Benthic segments, which are not present in the hydrodynamic network may nevertheless be included in the WASP5 network WASP5 segment numbering does not have to be the same as DYNHYD5 junction numbering Segments stacked vertically do not have to be numbered consecutively from surface water segments down

Once the network is set up, the model study will proceed through four general steps involving, in some manner, hydrodynamics, mass transport, water quality transformations, and environmental toxicology The first step addresses the question of where the water goes This can be answered by a combination of gaging, special studies, and hydrodynamic modeling Flow data can be interpolated or extrapolated using the principle of continuity Very simple flow routing models can be used very complicated multi-dimensional hydrodynamic models can also be used with proper averaging over time and space At present, the most compatible hydrodynamic model is DYNHYD5

The second step answers the question of where the material in the water is transported This can be answered by a combination of tracer studies and model calibration Dye and salinity are often used as tracers

The third step answers the question of how the material in the water and sediment is transformed and what its fate is This is the main focus of many studies Answers depend on a combination of laboratory studies, field monitoring parameter estimation calibration, and testing The net result is sometimes called model validation or verification, which are elusive concepts The success of this step depends on the skill of the user who must combine specialized knowledge with common sense and skepticism into a methodical process

The final step answers the question of how this material is likely to affect anything of interest, such as people, fish or the ecological balance Often, predicted concentrations are simply compared with water quality criteria adopted to protect the general aquatic community Care must be taken to insure that the temporal and spatial scales assumed in developing the criteria are compatible with those predicted by the model Sometimes principles of physical chemistry or pharmacokinetics are used to predict chemical body burdens and resulting biological effects The biaccumulation model FGETS (Suarez et al 1991) is a good example of this

CHAPTER 2

CHEMICAL TRACER TRANSPORT

2 1 MODEL DESCRIPTION

Introduction

A chemical tracer is a nonreactive chemical that is passively transported throughout the water body Examples include salinity or chlorides Special dyes are used as tracers although these often decay at a slow rate Setting up and calibrating a tracer is the first step in simulating more complex water quality variables.

Overview of WASP5 Tracer Transport

A conservative tracer is generally simulated using the TOXI5 program TOXI5 simulates the transport and transformation of one to three chemicals and one to three types of solids classes (Table 2 1) To simulate a tracer, the user should bypass solids and simulate chemical 1 with no decay A tracer is affected by transport, boundary and loading processes only as described below

Table 2 1 WASP5 State Variables for Toxicants

SYSTEM	VARIABLE
1	CHEMICAL 1
2	SOLIDS 1
3	SOLIDS 2
4	SOLIDS 3
5	CHEMICAL 2
6	CHEMICAL 3

WASP5 uses a mass balance equation to calculate chemical mass and concentrations for every segment in a specialized network that may include surface water, underlying water, surface bed, and underlying bed Simulated chemicals undergo several transport processes as specified by the user in the input dataset Chemicals are advected and dispersed among water segments, and exchanged with surficial benthic segments by dispersive mixing Dissolved chemicals migrate downward or upward through percolation and pore water diffusion.

The transport boundary, and loading processes for tracer chemicals are described below These same processes are also applied to the water quality variables desribed in subsequent chapters

Transport Processes

Water Column Advection

Advective water column flows directly control the transport of dissolved and particulate pollutants in many water bodies In addition, changes in velocity and depth resulting from variable flows can affect such kinetic processes as reaeration, volatilization, and photolysis An important early step in any modeling study is to describe or simulate water column advection properly In WASP5, water column flow is input via transport field one in Data Group D Circulation patterns may be described (flow options 1 and 2) or simulated by a hydrodynamic model such as DYNHYD5 (flow option 3) Flow options are specified in the first record of Data Group D

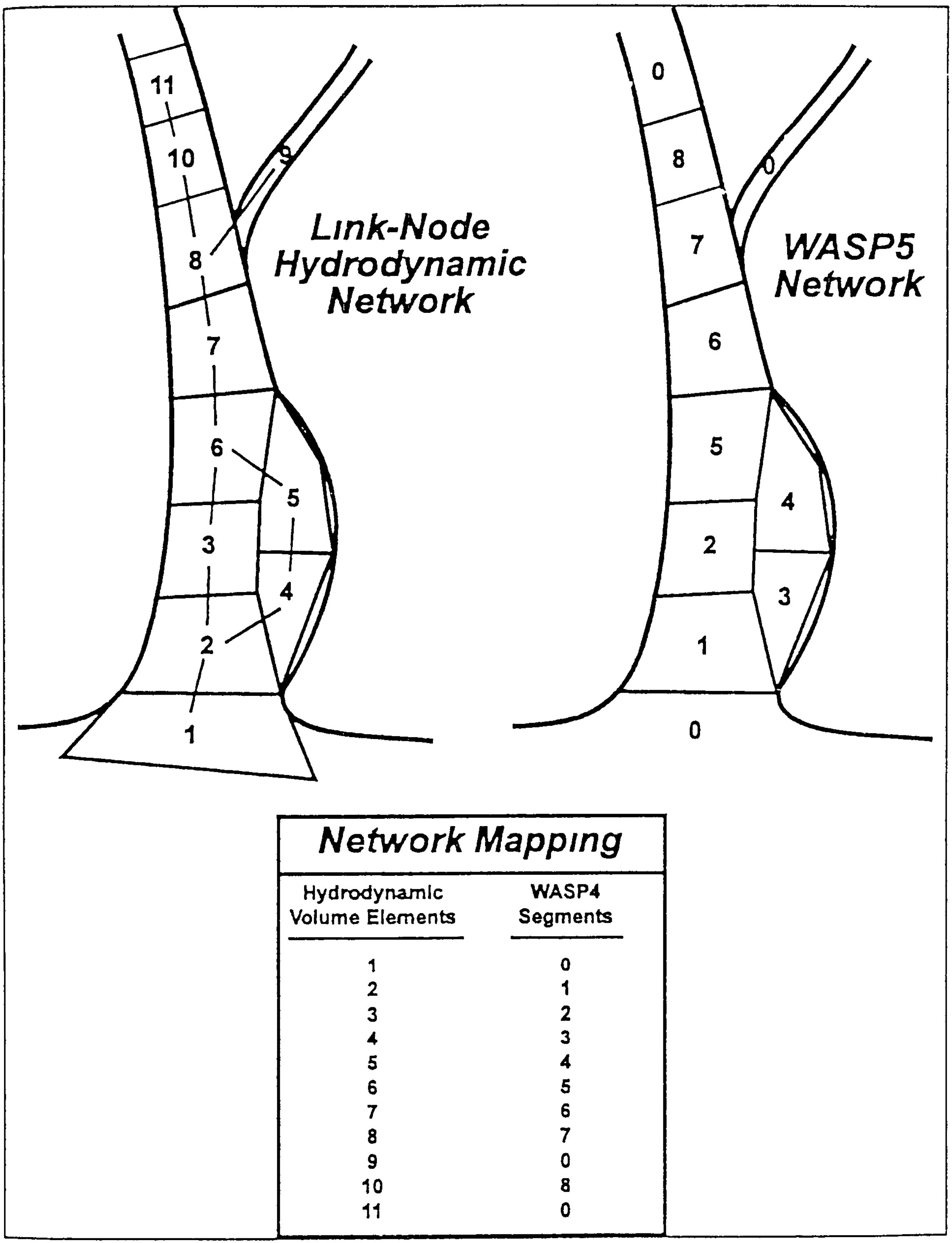
For descriptive flows, WASP5 tracks each separate inflow specified by the user from its point of origin through the model network For each inflow the user must supply a continuity or unit flow response function and a time function The time function describes the inflow as it varies in time The continuity function describes the unit flow response as it varies throughout the network The actual flow between segments that results from the inflow is the product of the time function and the continuity function

If several inflow functions are specified, then the total flow between segments is the sum of the individual flow functions Segment volumes are adjusted to maintain continuity In this manner, the effect of several tributaries, density currents, and wind-induced gyres can be described

In flow option 1 WASP5 sums all the flows at a segment interface to determine the direction of net flow, and then moves mass in the ONE direction In flow option 2 WASP5 moves mass independently of net flow, For example, if opposite flows are specified at an interface WASP5 will move mass in BOTH directions This option allows the user to describe large dispersive circulation patterns

Hydrodynamic Linkage

For unsteady flow in long networks, lag times may become significant and hydrodynamic simulations may be necessary to obtain sufficient accuracy Realistic simulations of unsteady transport can be accomplished by linking WASP5 to a compatible hydrodynamic simulation This linkage is accomplished through an



Network Mapping

Hydrodynamic Volume Elements	WASP4 Segments
1	0
2	1
3	2
4	3
5	4
6	5
7	6
8	7
9	0
10	8
11	0

Figure 2 1 Link-node hydrodynamic linkage

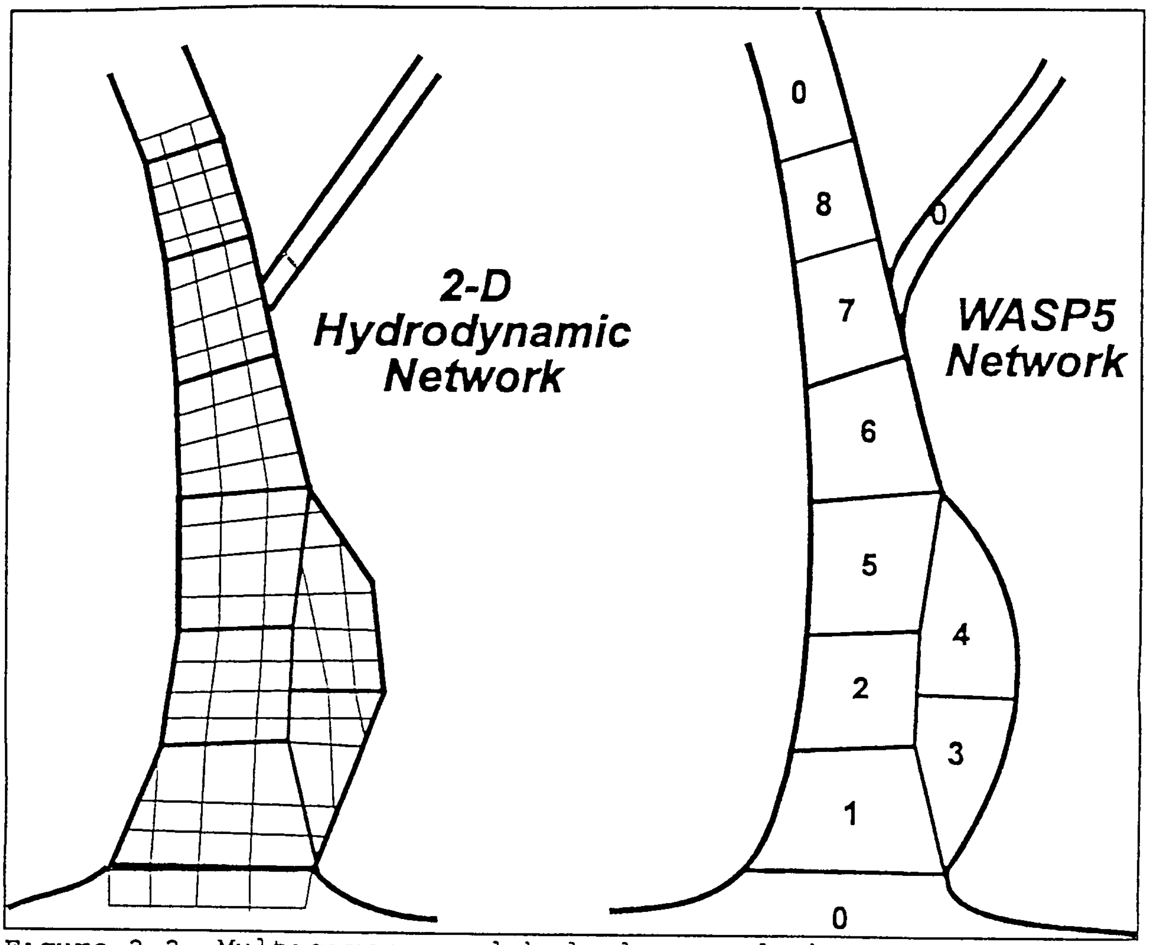


Figure 2 2 Multidimensional hydrodynamic linkage

external file chosen by the user at simulation time The hydrodynamic file contains segment volumes at the beginning of each time step, and average segment interfacial flows during each time step WASP5 uses the interfacial flows to calculate mass transport and the volumes to calculate constituent concentrations Segment depths and velocities may also be contained in the hydrodynamic file for use in calculating reaeration and volatilization rates

The first step in the hydrodynamic linkage is to develop a hydrodynamic calculational network that is compatible with the WASP5 network The easiest linkage is with link-node hydrodynamic models that run on equivalent spatial networks An example is given in Figure 2 1 Note that each WASP5 segment corresponds exactly to a hydrodynamic volume element or node Each WASP5 segment interface corresponds exactly to a hydrodynamic link, denoted in the figure with a connecting line

The hydrodynamic model calculates flow through the links and volume within the nodes Within the hydrodynamic model, the user must specify the water quality time step, or the number of hydrodynamic time steps per water quality time step The hydrodynamic model must then write out node volumes at the beginning of each water quality time step, and average link flows during each water quality time step A network map such as the one in Figure 2 1 must be supplied by the user in the hydrodynamic model or in an external interface program This map is used to create a hydrodynamic file that WASP5 can read and interpret The hydrodynamic model DYNHYD5, supplied with WASP5, contains subroutines to produce a proper WASP5 hydrodynamic file

It is important to note that the hydrodynamic model has additional nodes outside of the WASP5 network These additional nodes correspond to WASP5 boundaries, denoted by nominal segment number "0 " These extra hydrodynamic nodes are necessary because while flows are calculated only within the hydrodynamic network WASP5 requires boundary flows from outside its network

Multidimensional hydrodynamic models can also be linked to WASP5 A compatible two-dimensional network is illustrated in Figure 2 2 For the beginning of each water quality time step, the volumes within a WASP5 segment must be summed and written to the hydrodynamic file For the duration of each water quality time step, flows across the WASP5 segment boundaries must be averaged All of the averaged flows across a boundary must then be summed and written to the hydrodynamic file Again it is important to note the presence of hydrodynamic elements outside the WASP5 network generating boundary flows

To implement the hydrodynamic linkage, the user must specify flow option 3 in the input dataset If IQOPT is set to 3 a menu of previously prepared hydrodynamic files (* HYD) is presented Following the choice of a proper file the simulation time step will be reset by the hydrodynamic file The time steps read in Data Group A will be ignored Similarly, water column segment volumes will be read from the hydrodynamic file The user must nevertheless enter a time step and volumes for each segment in the usual location During the simulation flows and volumes are read every time step

The contents and format of the hydrodynamic file are detailed in Part B The WASP5 Input Dataset Section 5 2

Hydraulic Geometry

A good description of segment geometry as a function of flow conditions can be important in properly using WASP5 to simulate rivers For flow option 3 velocity and depth are computed within the hydrodynamic model, and are read by WASP5 For flow options 1 and 2, a set of user-specified hydraulic discharge coefficients from Data Group C defines the relationship between velocity, depth and stream flow in the various segments This method, described below, follows the implementation in QUAL2E (Brown and Barnwell, 1987) In WASP5, these segment velocities and depths are only used for calculations of reaeration and volatilization rates, they are not used in the transport scheme

Discharge coefficients giving depth and velocity from strea flow are based on empirical observations of the stream flow relationship with velocity and depth (Leopold and Maddox, 1953) It is important to note that these coefficients are only important when calculating reaeration or volatilization The velocity calculations are not used in time of travel and will not affect the simulation of tracers The equations relate velocity, channel width, and depth to streamflow through power functions

$$V = a\,Q^{b} \qquad 2\ 1$$

$$D = c\,Q^{d} \qquad 2\ 2$$

$$B = e\,Q^{f} \qquad 2\ 3$$

where

D is average depth, m

B is average width, m

a, b c d e and f are empirical coefficients or exponents

Given that area is a function of average width (B) and average depth (D)

$$A = D\,B \qquad 2\ 4$$

it is clear from continuity that

$$Q = U\,A = U\,D\,B = (aQ^{b})\ (cQ^{d})\ (eQ^{f}) = (a\ c\ e)\,Q^{b+d+f} \qquad 2\ 5$$

and therefore, the following relationships hold

$$a c e = 1 \qquad 2\ 6$$

$$b + d + f = 1 \qquad 2\ 7$$

WASP5 only requires specification of the relationships for velocity Equation 2 1 and depth Equation 2 2, the coefficients for Equation 2 3 are implicitly specified by Equations 2 6 and 2 7

These options can be put into perspective by noting that, for a given specific channel cross-section, the coefficients (a, c e) and exponents (b, d f) can be derived from Mannings equation For example, if a channel of rectangular cross-section is assumed, then width (B) is not a function of streamflow (Q) the exponent (f) is zero (0 00) and the coefficient (e) is the width of the rectangular channel (B) By noting that hydraulic radius (R) is approximately equal to depth (D) for wide streams and that A = D B the discharge coefficients for rectangular cross sections can be shown to be 0 4 for velocity and 0 6 for width

Leopold et al (1964) have noted that stream channels in humid regions tend towards a rectangular cross-section because cohesive soils promote steep side slopes whereas noncohesive soils encourage shallow sloped almost undefined banks

Table 2 2 Comparison of Hydraulic Exponents

Channel Cross-Section	Exponent for (b) Velocity	Exponent for (d) Depth	Exponent for (f) Width
Rectangular	0 40	0 60	0 00
Average of 158 U S Gaging Stations	0 43	0 45	0 12
Average of 10 Gaging Stations on Rhine River	0 43	0 41	0 13
Ephemeral Streams in Semiarid U S	0 34	0 36	0 29

Table 2 2 compares hydraulic exponents for a rectangular channel with data reported by Leopold et al (1964) Note that the average velocity exponent is relatively constant for all channel cross sections The major variation occurs as a decrease in the depth exponent and concomitant increase in the width exponent as channel cross-sections change from the steep side slopes characteristic of cohesive soils to the shallow slopes of arid regions with noncohesive soils

For bodies of water such as ponds, lakes, and reservoirs, velocity and depth may not be a function of flow For these cases, both the velocity and depth exponents (b and d) can be chosen to be zero (0 00) Because Q to the zero power is equal to one (1 0), the coefficients a and c must be the velocity and depth, i e ,

IF b = 0 0 THEN a = V, and

IF d = 0 0 THEN c = D

When the depth exponent is zero, WASP5 will adjust segment depths with segment volumes assuming rectangular sides

For site-specific river or stream simulations hydraulic coefficients and exponents must be estimated Brown and Barnwell (1987) recommended estimating the exponents (b and d) and then calibrating the coefficients (a and c) to observed velocity and depth The exponents may be chosen based on observations of channel shape noted in a reconnaissance survey If cross sections are largely rectangular with vertical banks, the first set of exponents shown in Table 2 2 should be useful If channels have steep banks typical of areas with cohesive soils then the second set of exponents is appropriate If the stream is in an arid region with typically noncohesive soils and shallow sloping banks then the last set of exponents is recommended

The key property of the channel that should be noted in a reconnaissance survey is the condition of the bank slopes or the extent to which width would increase with increasing streamflow Clearly the bank slopes and material in contact with the streamflow at the flow rate(s) of interest are the main characteristics to note in a reconnaissance Table 2 2 gives general guidance but it should be noted that values are derived for bankful flows Even in streams with vertical banks the low flows may be in contact with a sand bed having shallow sloped almost nonexistent banks more representative of ephemeral streams in semi-arid areas

Pore Water Advection

Pore water flows into or out of the bed can significantly influence benthic pollutant concentrations Depending on the direction of these flows and the source of the pollutants, pore water advection may be a source or sink of pollutants for the overlying water column

If benthic segments are included in the model network the user may specify advective transport of dissolved chemicals in the pore water In WASP5 pore water flows are input via transport field two Pore water advection transports water and dissolved chemical sediment and particulate chemical are not transported The mass derivative of chemical due to pore water flow from segment j to segment i is given by

$$\frac{\partial M_{ik}}{\partial t} = Q_{ji}\, f_{Dj}\, C_{jk}/n_j \qquad 2.8$$

where

M = mass of chemical k in segment i, g

C_{jk} = total concentration of chemical 'k in segment "j," mg/L (g/m^3)

n_j = porosity of segment j, L_w/L

f_{Dj} = dissolved fraction of chemical in segment

Q_{ji} = pore water flow rate from j to i, m^3/day

Dissolved fractions f_D may be input by the user in Data Group J In TOXI5 these are recomputed from sorption kinetics each time step

WASP5 tracks each separate pore water inflow through the benthic network For each inflow (or outflow), the user must supply a continuity function and a time function The actual flow through benthic segments that results from each inflow is a product of the time function and the continuity function If a flow originates in or empties into a surface water segment then a corresponding surface water flow function must be described in flow field 1 that matches the pore water function

Water Column Dispersion

Dispersive water column exchanges significantly influence the transport of dissolved and particulate pollutants in such water bodies as lakes reservoirs and estuaries Even in rivers longitudinal dispersion can be the most important process diluting peak concentrations that may result from unsteady loads or spills Natural or artificial tracers such as dye, salinity, or even heat are often used to calibrate dispersion coefficients for a model network

In WASP5, water column dispersion is input via transport field one in Data Group B Several groups of exchanges may be defined by the user For each group, the user must supply a time function giving dispersion coefficient values (in m^2/sec) as they vary in time For each exchange in the group the user must supply an interfacial area, a characteristic mixing length, and the adjoining segments between which the exchange takes place The characteristic mixing length is typically the distance between the segment midpoints The interfacial area is the area normal to the characteristic mixing length shared by the exchanging segments (cross-sectional area for horizontal exchanges or surface area for vertical exchanges) The actual dispersive exchange between segments i and j at time t is given by

$$\frac{\partial M_{ik}}{\partial t} = \frac{E_{ij}(t)\ \ A_{ij}}{L_{cij}} (C_{jk} - C_{ik}) \qquad 2\ 9$$

where

M_{ik} = mass of chemical "k in segment 'i " g

C_{ik} C_{jk} = concentration of chemical k in segment i and 'j,' mg/L (g/m^3)

$E_{ij}(t)$ = dispersion coefficient time function for exchange 'ij' m^2/day

A_{ij} = interfacial area shared by segments 'i and j," m^2

L_{cij} = characteristic mixing length between segments i and j m

Pore Water Diffusion

Diffusive pore water exchanges can significantly influence benthic pollutant concentrations particularly for relatively soluble chemicals and water bodies with little sediment loading Depending on the dissolved concentration gradient, pore water diffusion may be a source or sink of pollutants for the overlying water column

If benthic segments are included in the model network the user may specify diffusive transport of dissolved chemicals in the pore water In WASP5, pore water diffusion is input via transport field two in Data Group B Several groups of exchanges may be defined by the user

For each exchange group the user must supply a time function giving dispersion coefficient values (in m^2/sec) as they vary in time For each exchange in the group, the user must supply an interfacial area, a characteristic mixing length, and the segments between which exchange takes place The characteristic mixing length is typically the distance between two benthic segment midpoints (multiplied internally by the tortuosity, which is roughly the inverse of porosity) For pore water exchange with a surface water segment, (the characteristic mixing length) is usually taken to be the depth of the surficial benthic segment The interfacial area is the surficial area of the benthic segment (which is input by the user) multiplied internally by porosity

There may be several surficial benthic segments underlying a water column segment representing discrete benthic deposits (or habitats) The concentration of chemical diffusing is the dissolved fraction per unit pore water volume The actual diffusive exchange between benthic segments i and j at time t is given by

$$\frac{\partial M_{ik}}{\partial t} = \frac{E_{ij}(t)\ A_{ij}\ n_{ij}}{L_{cij}/n_{ij}} \left(\frac{f_{Djk}\ C_{jk}}{n_j} - \frac{f_{Dik}\ C_{ik}}{n_i} \right) \qquad 2\ 10$$

where

f_{Dik} f_{Djk} = dissolved fraction of chemical "k in segments i and j

n_i = average porosity at interface ij L_w/L

$E_{ij}(t)$ = diffusion coefficient time function for exchange "ij" m^2/day

A_{ij} = interfacial area shared by segments 'i and 'j " m^2

L_{cij} = characteristic mixing length between segments "i and j,' m

Boundary Processes

A boundary segment is characterized by water exchanges from outside the network, including tributary inflows downstream outflows, and open water dispersive exchanges WASP5 determines its boundary segments by examining the advective and dispersive segment pairs specified by the user If an advective or dispersive segment pair includes segment number "0 " the other segment number is a boundary segment Thus, for advective flows, the segment pair (0,1) denotes segment 1 as an upstream boundary segment segment pair (5,0) denotes segment 5 as a downstream boundary segment

Boundary concentrations C_{Bik} (mg/L) must be specified for each simulated variable "k" at each boundary segment 'i" These concentrations may vary in time At upstream boundary segments, WASP5 applies the following mass loading rates

$$V_i S_{Bik} = Q_{0i}(t) \quad C_{Bik} \qquad 2\ 11$$

where

S_{Bik} = boundary loading rate response of chemical k in segment i g/m^3-day

V = volume of boundary segment "i " m^3

Q (t) = upstream inflow into boundary segment i," m /day

At downstream boundary segments WASP5 applies the following mass loading rates

$$V_i S_{Bik} = -Q_{i0}(t) \quad C_{ik} \qquad 2\ 12$$

where

$Q_{0}(t)$ = downstream outflow from boundary segment 'i m /day

C_{ik} = internal concentration of chemical k in segment i mg/L

Notice that the specified boundary concentration is not used to calculate the boundary loading rate for the downtream boundary segment If however the downstream outflow becomes negative, it becomes in reality an inflow In this case Equation 2 11 applies where Q_{0i} = $-Q_{i0}$

At exchange boundary segments, WASP5 applies the following mass loading rates

$$V_i S_{Bi} = \frac{E_{io}(t) \quad A_{io}}{L_{cio}} \left(C_{Bk} - C_{ik}\right) \qquad 2\ 13$$

where terms are as defined above When a boundary concentration exceeds the internal concentration, mass is added to the boundary segment when the boundary concentration falls below the internal concentration mass is lost from the boundary segment

Loading Processes

WASP5 allows the user to specify loading rates for each variable Two types of loadings are provided for -- point source loads and runoff loads The first set of loads is specified by the user in the input dataset The second set of loads is read by WASP5 from a nonpoint source loading file created by an appropriate loading model Both kinds of loads in kg/day, are added to the designated segments at the following rates

$$V_i S_{Lik} = 1000 \quad L_{ik}(t) \qquad 2\ 14$$

where

S_{Lik} = loading rate response of chemical k in segment i, g/m^3-day

$L_{ik}(t)$ = loading rate of chemical k into segment i kg/day

Point source loads are input as a series of loading versus time values During a simulation WASP5 interpolates between these points to provide time-variable loadings The WASP5 calculational time step should be set by the user to a value that is divisible into the difference in time entries in the point source loading functions If evenly divisible time steps cannot be specified, the user should specify maximum time steps at least 5 times smaller than the point source time entries If the user is specifying daily load variations, for example, the maximum time step should be 0 2 days

The user should understand that mass entered as loads is not directly accompanied with inflow No significant errors are introduced if the inflow associated with a loading is small compared with the water body flow If a loading is associated with significant inflow, then the user should generally enter the associated flows separately under water column advection, and treat the loading as a model boundary by specifying the boundary concentration accompanying the inflow If a large number of diffuse loads are being read in, the user can provide for the incremental flows using a flow continuity function that increases downstream

Nonpoint Source Linkage

Realistic simulations of nonpoint source loadings can be accomplished by linking WASP5 to a compatible surface runoff simulation This linkage is accomplished through a formatted external file chosen by the user at simulation time The nonpoint source loading file contains information on which WASP5 systems and segments receive nonpoint source loads, and a record of the nonzero loads by system segment, and day

If the user sets the nonpoint source loading flag (Data Group F, Record 5) to 1, a menu of previously prepared nonpoint source files (* NPS) is presented Following the choice of a proper file, nonpoint source loads are read once a day throughout a simulation from a loading file generated by a previous loading model simulation These loads are treated as step functions that vary daily When the user implements the nonpoint source loading option, model time steps should be divisible into 1 day (Time steps do not have to be exactly divisible into a day if time steps are small, any errors associated with carrying the previous day's loading rate into a new day will be small)

The contents and format of the nonpoint source file are detailed in Part B The WASP5 Input Dataset Section 7 2

Initial Conditions

Because WASP5 is a dynamic model the user must specify initial conditions for each variable in each segment Initial conditions include the chemical concentrations at the beginning of the simulation The product of the initial concentrations and the initial volumes give the initial constituent masses in each segment For steady simulations, where flows and loadings are held constant and the steady-state concentration response is desired, the user may specify initial concentrations that are reasonably close to what the final concentrations should be For dynamic simulations where the transient concentration response is desired, initial concentrations should reflect measured values at the beginning of the simulation

In addition to chemical concentrations, the dissolved fractions must be specified for each segment at the beginning of the simulation For tracers, the dissolved fractions will normally be set to 1 0 For tracers, as well as dissolved oxygen, eutrophication, and sediment transport, the initial dissolved fractions remain constant throughout the simulation For organic chemical simulations, the dissolved fraction will be internally calculated from partition coefficients and sediment concentrations

The density of each constituent must be specified under initial conditions For tracers, this value should be set to 1 0

2 2 MODEL IMPLEMENTATION

Introduction

To simulate a tracer with WASP5, use the preprocessor or text editor to create a TOXI5 input file The preprocessor will create an input file with parameters in the proper fields Using a text editor, the user must take care to enter parameters into the proper fields A general description of the input dataset is given in Part B of this document The model input parameters are organized below as they are presented in the preprocessor The data group, record number, and input parameter name are also given for reference

Model Input Parameters

This section summarizes the input parameters that must be specified in order to solve the WASP5 mass balance equation Input parameters are prepared for WASP5 in four major sections of the preprocessor -- environment, transport, boundaries, and transformations

Environment Parameters

These parameters define the basic model identity, including the segmentation and control the simulation

Simulation Type-- The user must specify which WASP5 model will be run with the dataset The present choices are 'TOXI4 or EUTRO4 (Group A Record 1, SIMTYP)

Simulation Titles-- The user may specify a 2-line title for the simulation This title may include any descriptive information on the water body, time frame, pollutants, simulation parameters etc The user may also specify the properly positioned names of the simulation switches input in Record 4 This is for user convenience only (Group A Records 1 2, 3 TITLE1, TITLE2, HEADER)

Number of Segments-- The user must specify the number of segments in the model network (Group A, Record 4 NOSEC)

Number of Systems-- The user must specify the number of model systems (state variables) in the simulation In the preprocessor select "simulate" for Chemical 1, and bypass" for Chemicals 2 and 3 and Solids 1-3 For bypassed variables, the bypass option SYSBY(I) is set to 1 (Group A, Record 4, NOSYS, Record 10 SYSBY(I))

Restart Option-- The user must specify the restart option, which controls the use of the simulation restart file This restart file stores the final conditions from a simulation, and can be used to input initial conditions in a sequential simulation 0 = neither read from nor write to the restart file 1 = write final simulation results to restart file, 2 = read initial conditions from restart file created by earlier simulation, and write final simulation results to new restart file (Group A, Record 4 ICFL)

Message Flag-- The user must specify the option controlling messages printed to screen during the simulation 0 = all messages printed, including data input and simulated concentrations 1 = simulated concentrations only printed 2 = no messages printed to screen (Group A Record 4 MFLG)

Mass Balance Analysis-- The user should specify the system number for which a global mass balance analysis will be performed A value of 0 will result in no mass balance table being generated (Group A, Record 4, JMAS)

Negative Solution Option-- Normally, concentrations are not allowed to become negative If a predicted concentration at t + Δt is negative, WASP maintains its positive value by instead halving the concentration at time t The negative solution option lets the user bypass this procedure allowing negative concentrations This may be desirable for simulating dissolved oxygen deficit in the benthos, for example 0 = prevents negative concentrations, 1 = allows negative concentrations (Group A, Record 4 NSLN)

Time Step Option-- The user must specify how time steps will be determined during the simulation 0 = user inputs time step history 1 = model calculates time step (Group A Record 4 INTY)

Advection Factor, dimensionless-- The advection factor υ can be specified to modify the finite difference approximation of $\partial c/\partial x$ used in the advection term by WASP For $\upsilon = 0$ the backward difference approximation is used This is most stable and is recommended for most applications For $\upsilon = 0\ 5$, the central difference approximation is used This is unstable in WASP, and is not recommended

Table 2 3 Values of Numerical Dispersion (m^2/sec)

	U (m/sec)					
υ	0 1	0 2	0 4	0 6	0 8	1 0
			Δt = 1000 sec			
0 0	95	180	320	420	480	500
0 1	75	140	240	300	320	300
0 2	55	100	160	180	160	100
0 3	35	60	80	60	0	--
0 4	15	20	0	--	--	--
			Δt = 2000 sec			
0 0	90	160	240	240	160	0
0 1	70	120	160	120	0	--
0 2	50	80	80	0	--	--
0 3	30	40	0	--	--	--
0 4	10	0	--	--	--	--
			Δt = 4000 sec			
0 0	80	120	80	--	--	--
0 1	60	80	0	--	--	--
0 2	40	40	--	--	--	--
0 3	20	0	--	--	--	--
0 4	0	--	--	--	--	--
			Δt = 8000 sec			
0 0	60	40	--	--	--	--
0 1	40	0	--	--	--	--
0 2	20	--	--	--	--	--
0 3	0	--	--	--	--	--
0 4	--	--	--	--	--	--

A nonzero advection factor is helpful in situations where the network size and time step produce large numerical dispersion A nonzero advection factor reduces the numerical dispersion produced by a particular velocity, length, and time step combination According to Bella and Grenney (1970)

$$E_{num} = \frac{U}{2} [(1-2\nu) L - U \Delta t] \qquad 2\ 15$$

Note that a ν of 0 reduces this to Equation 2 20 Values of E_{num} for a length of 2000 meters and various combinations of velocity and time step are provided in Table 2 3 For a particular velocity, say 0 4 m/sec, numerical dispersion can be reduced by increasing the time step For ν = 0, increasing the time step from 1000 to 4000 seconds decreases E_{num} from 320 to 80 m^2/sec If the time step must be 1000 seconds however numerical dispersion can still be reduced by increasing ν In this case, increasing ν from 0 to 0 4 decreases E_{num} from 320 to 0 m^2/sec (Group A, Record 4, ADFC)

Initial Time, day, hour, minute-- The time at the beginning of the simulation must be specified in order to synchronize all the time functions The day hour and minute can be input The beginning of the simulation is day 1 (Group A, Record 4 ZDAY, ZHR, ZMIN)

Final Time, days--The elapsed time at the end of the simulation must be specified in days (including decimal fraction) The end of the simulation occurs when the final time from the integration time step history is encountered The final time is entered on the same record as the time step (Group A Record 7 T(NOBRK))

Transport Analysis Flag-- The user should specify whether the transport analysis file will be generated during the simulation A value of 0 causes the file to be generated a value of 1 prevents the file from being generated (Group A Record 4 TFLG)

Runtime Display Segments-- The user must specify up to six segments for display on the screen during the simulation Concentrations in these segments will be written and updated on the screen These segments can be changed during the simulation (Group A Record 5, ISEGOUT)

Integration Time Step, days--A sequence of integration time steps (Δt) must be specified, along with the time interval over which they apply If time step option (INTY) was set to 0 these time steps will be used during the simulation If the time step option was set to 1, the model will calculate time steps internally the time steps given here are the maximum allowed

Given specific network and transport parameters time steps are constrained within a specific range to maintain stability and minimize numerical dispersion, or solution inaccuracies To maintain stability at a segment the advected, dispersed, and transformed mass must be less than the resident mass

$$\Sigma\ Q\ C_j + \Sigma\ R\ C_j + \Sigma\ S_K\ V_j)\ \Delta t < V_j\ C_j \qquad 2\ 16$$

[illegible]

Solving for Δt and applying the criterion over the entire network with appropriate factors gives the maximum stable step size used by WASP5

$$\Delta t_{max} = 0\ 9\ Min\left(\frac{V_j}{\sum_i Q_{ij} + \sum_i R_{ij} + 5\sum_k (S_{Kjk}\ V_j / C_j)}\right) \qquad 2\ 17$$

For purely advective systems, Equation 2 17 sets the time step to 90% of the minimum segment travel time For purely dispersive systems, Equation 2 17 sets the time step to 90% of the minimum segment flushing time For a linear reactive system with no transport Equation 2 17 sets the time step to 18% of the reaction time Usually Δt is controlled by advective or dispersive flows

Numerical dispersion is artificial mixing caused by the finite difference approximation used for the derivatives If the advection factor $\upsilon = 0$, the backward difference approximation of $\partial c/\partial x$ is used in the advection term, and

$$E_{num} = \frac{U\ L}{2} \qquad 2\ 18$$

where

L = length of the segment m

For the Euler scheme the forward difference approximation of $\partial c/\partial t$ is used, and

$$E_{num} = \frac{U^2\ \Delta t}{2} \qquad 2\ 19$$

The total numerical dispersion, then is

[illegible]

Note that increas~~ing the~~ time step up to Δx/U (or V/Q)

$$E_{num} = \frac{U}{2} (L - U \Delta t) \tag{2 20}$$

decreases numerical dispersion to 0 The conditions for stability discussed above require a time step somewhat less than V/Q for most segments So to maintain stability and minimize numerical dispersion in a water body subject to unsteady flow, the sequence of time steps must be as large as possible, but always less than Δt_{max} given in Equation 2 17 (Group A, Record 6, NOBRK Record 7, DTS, T)

Print Intervals, days-- The user must specify the print intervals controlling the output density in the print file transferred to the post-processor The model will store all display variables in all segments after each print interval throughout the simulation Different print intervals can be specified for different phases in the simulation At least two print intervals must be specified, one for time 0 and one for the final time NPRINT is the number of different print intervals to input PRINT(I) is the print interval to be used until time TPRINT(I) TPRINT(I) is the time up to when print interval PRINT(I) will be used (Group A, Record 8 NPRINT Record 9 PRINT(I) TPRINT(I))

Segment Volumes, m^3--Initial volumes for each segment must be specified These can be calculated from navigation charts or from a series of transects measuring depth versus width along the river Sometimes, volumes can be estimated from the travel time of a well-mixed cloud of dye through a reach For simulations using hydrodynamic results from DYNHYD5, volumes from the hydrodynamic summary file (* HYD) are used and continuity is maintained (Group C Record 3, BVOL(ISEG))

Transport Parameters

This group of parameters defines the advective and dispersive transport of simulated model variables Input parameters include advective flows sediment transport velocities, dispersion coefficients cross-sectional areas and characteristic lengths Although the nominal units expected by the model are SI, English or other units can be used along with proper specification of conversion factors

Number of Flow Fields-- Under advection, the user has a choice of up to six flow fields To simulate surface water transport select water column flow in the preprocessor or set the number of flow fields to 1 When simulating pore water flow, select this option in the preprocessor or set the number of flow fields to 2 (Group D, Record 1, NFIELD)

Advective Flow, m^3/sec--Steady or unsteady flows can be specified between adjoining segments, as well as entering or leaving the network as inflow or outflow The user must be careful to check for continuity errors, as the model does not require that flow continuity be maintained For example the user may specify that more flow enters a segment than leaves For simulations using hydrodynamic results from DYNHYD5 flows from the * HYD file are used and flow continuity is automatically maintained (Group D, Record 4, BQ Record 6, QT(K), TQ(K))

Number of Exchange Fields-- Under dispersion, the user has a choice of up to two exchange fields To simulate surface water toxicant and solids dispersion, select water column dispersion in the preprocessor or set the number of exchange fields to 1 To simulate exchange of dissolved toxicants with the bed, the user should also select pore water diffusion in the preprocessor or set the number of exchange fields to 2 (Group B, Record 1, NRFLD)

Dispersion Coefficients, m^2/sec--Dispersive mixing coefficients can be specified between adjoining segments, or across open water boundaries These coefficients can model pore water diffusion in benthic segments, vertical diffusion in lakes and lateral and longitudinal dispersion in large water bodies Values can range from 10 m^2/sec for molecular diffusion to $5x10^2$ m^2/sec for longitudinal mixing in some estuaries Values are entered as a time function series of dispersion and time in days (Group B, Record 6 RT(I), TR(I))

Cross-Sectional Area, m^2--Cross-sectional areas are specified for each dispersion coefficient, reflecting the area through which mixing occurs These can be surface areas for vertical exchange such as in lakes or in the benthos Areas are not modified during the simulation to reflect flow changes (Group B Record 4, A(K))

Characteristic Mixing Length, m--Mixing lengths are specified for each dispersion coefficient reflecting the characteristic length over which mixing occurs These are typically the lengths between the center points of adjoining segments A single segment may have three or more mixing lengths for segments adjoining longitudinally, laterally and vertically For surficial benthic segments connecting water column segments the depth of the benthic layer is a more realistic mixing length than half the water depth (Group B Record 4, EL(K))

Boundary Parameters

This group of parameters includes boundary concentrations waste loads, and initial conditions Boundary concentrations must be specified for any segment receiving flow inputs, outputs, or exchanges Initial conditions include not only initial concentrations, but also the density and solids transport field for each solid, and the dissolved fraction in each segment

Boundary Concentrations, mg/L--Steady or time-variable concentrations must be specified for each water quality constituent at each boundary A boundary is either a tributary inflow, a downstream outflow, or an open water end of the model network across which dispersive mixing can occur Advective and dispersive flows across boundaries are specified by the transport parameters Values are entered as a time function series of concentrations and time, in days (Group E, Record 4 BCT(K), T(K))

Waste Loads, kg/day--Steady or time-variable loads may be specified for each water quality constituent at several segments These loads represent municipal and industrial wastewater discharges urban and agricultural runoff precipitation, and atmospheric deposition of pollutants Values are entered as a time function series of loads and time in days (Group F, Record 4, WKT(K) T(K))

Initial Concentrations, mg/L--Concentrations of each constituent in each segment must be specified for the time at which the simulation begins For those water bodies with low transport rates the initial concentrations of conservative substances may persist for a long period of time Accurate simulation, then would require accurate specification of initial concentrations If initial concentrations cannot be determined accurately, then longer simulations should be run and early predictions discounted (Croup J, Record 2, C(ISYS J))

Dissolved Fractions--The initial fraction of chemical dissolved in the water portion of a segment is input as a fraction of total chemical concentration The dissolved fraction is important in determining the amount of chemical transported by pore water flow and dispersion and by solids transport Dissolved fractions may be computed from sorption kinetics in the transformation subroutines (Group J, Record 2 DISSF(ISYS J))

Solid Densities, g/cm--The density of each type of solid is needed to compute the porosity of bed segments Porosity will be a function of sediment concentration and the density of each solid type (Group J Record 1, DSED(K))

Maximum Concentrations, mg/L--Maximum concentrations must be specified for each water quality constituent The simulation is automatically aborted if a calculated concentration falls outside these limits This usually indicates computational instability, and the time step must usually be reduced (Group J, Record 1 CMAX(K))

Transformation Parameters

This group of parameters includes spatially variable parameters, constants, and kinetic time functions for the water quality constituents being simulated None are necessary for dissolved, conservative chemicals

External Input Files

At the user's option, two external input files may be called upon and used by WASP5 during a simulation These formatted files may be created by a simulation model or by output from a spreadsheet As formatted ASCII files, they may be edited using standard text editors Hydrodynamic files are denoted by * HYD, where the user specifies a 1 to 8 character name for * Nonpoint source loading files are denoted by * NPS The contents and format for these files are specified in Part B, Sections 5 2 and 7 2

CHAPTER 3

SEDIMENT TRANSPORT

3 1 MODEL DESCRIPTION

Introduction

Sediment transport is potentially a very important process in aquatic systems Excess sediment can affect water quality directly Water clarity and benthic habitats can be degraded Sediment transport also influences chemical transport and fate Many chemicals sorb strongly to sediment and thus undergo settling, scour, and sedimentation Sorption also affects a chemical s transfer and transformation rates Volatilization and base-catalyzed hydrolysis for example, are slowed by sorption Both sediment transport rates and concentrations must be estimated in most toxic chemical studies

In general the stream transport capacity for suspended sediment is in excess of its actual load, and the problem is one of estimating sediment source loading--namely, watershed erosion (In areas of backwater behind dams or in sluggish reaches, the stream transport capacity may drop enough to allow net deposition) Strongly sorbed pollutants may build up ~~significantly~~ Because sediment transport can be complex, site-specific calibration of the settling, scour, and sedimentation rates is usually necessary

Overview of WASP5 Sediment Transport

Sediment size fractions or solids types, are simulated using the TOXI5 program Simulations may incorporate total solids as a single variable, or, alternately, represent from one to three solids types or fractions The character of the three solids types is user-defined They may represent sand silt and clay or organic solids and inorganic solids The user defines each solid type by specifying its settling and erosion rates and its organic content

WASP5 performs a simple mass balance on each solid variable in each compartment based upon specified water column advection and dispersion rates, along with special settling deposition erosion, burial, and bed load rates Mass balance computations are performed in benthic compartments as well as water column compartments Bulk densities or benthic volumes are adjusted throughout the simulation

All solids transport rates can be varied in space and time by the user There are, however, no special process descriptions for solids transport Erosion rates, for example, are not programmed as a function of sediment shear strength and water column shear stress Consequently, the TOXI5 sediment model should be considered descriptive, and must be calibrated to site data

Sediment Transport Processes

Water Column Transport

Sediment and particulate chemicals in the water column may settle to lower water segments and deposit to surficial bed segments Settling deposition, and scour rates in WASP5 are described by velocities and surface areas in transport fields 3, 4 and 5 Particulate transport velocities may vary both in time and in space and are multiplied by cross-sectional areas to obtain flow rates for solids and the particulate fractions of chemicals

Settling velocities should be set within the range of Stoke's velocities corresponding to the suspended particle size distribution

$$V_s = \frac{8\ 64\ g}{18\ \mu}(\rho_p - \rho_w)\ d_p^2 \qquad 3\ 1$$

where

V_s = Stokes velocity for particle with diameter d_p and density ρ_p, m/day

g = acceleration of gravity = 981 cm/sec^2

μ = absolute viscosity of water = 0 01 poise (g/cm^3-sec) at 20 [illegible]

ρ_p = density of the solid g/cm^3

ρ = density of water 1 0 g/cm^3

d_p = particle diameter, mm

Values of V_s for a range of particle sizes and densities are provided in Table 3 1

Benthic Exchange

Table 3 1 Stoke's Settling Velocities (in m/day) at 20 [illegible]

Particle Diameter, mm	Particle Density, g/cm 1 80	 2 00	 2 50	 2 70
Fine Sand				
0 3	300 00	400 00	710 00	800 00
0 05	94 00	120 00	180 00	200 00
Silt				
0 05	94 00	120 00	180 00	200 00
0 02	15 00	19 00	28 00	32 00
0 01	3 80	4 70	7 10	8 00
0 005	0 94	1 20	1 80	2 00
0 002	0 15	0 19	0 28	0 32
Clay				
0 002	0 15	0 19	0 28	0 32
0 001	0 04	0 05	0 07	0 08

Benthic exchange of sediment and particulate chemicals is driven by the net scour and deposition velocities

$$W_{BS} = A_{ij} \, (w_R \, S_i - w_D \, S_j) \qquad 3\ 2$$

where

W_{BS} = net sediment flux rate, g/day

S = sediment concentration, g/m^3

w_D = deposition velocity, m/day

w_R = scour velocity, m/day

A_{ij} = benthic surface area, m^2

i = benthic segment

j = water segment

The deposition velocity can be calculated as the product of the Stokes settling velocity and the probability of deposition

$$w_D = V_s \, \alpha_D \qquad 3.3$$

where

α_D = probability of deposition upon contact with the bed

The probability of deposition depends upon the shear stress

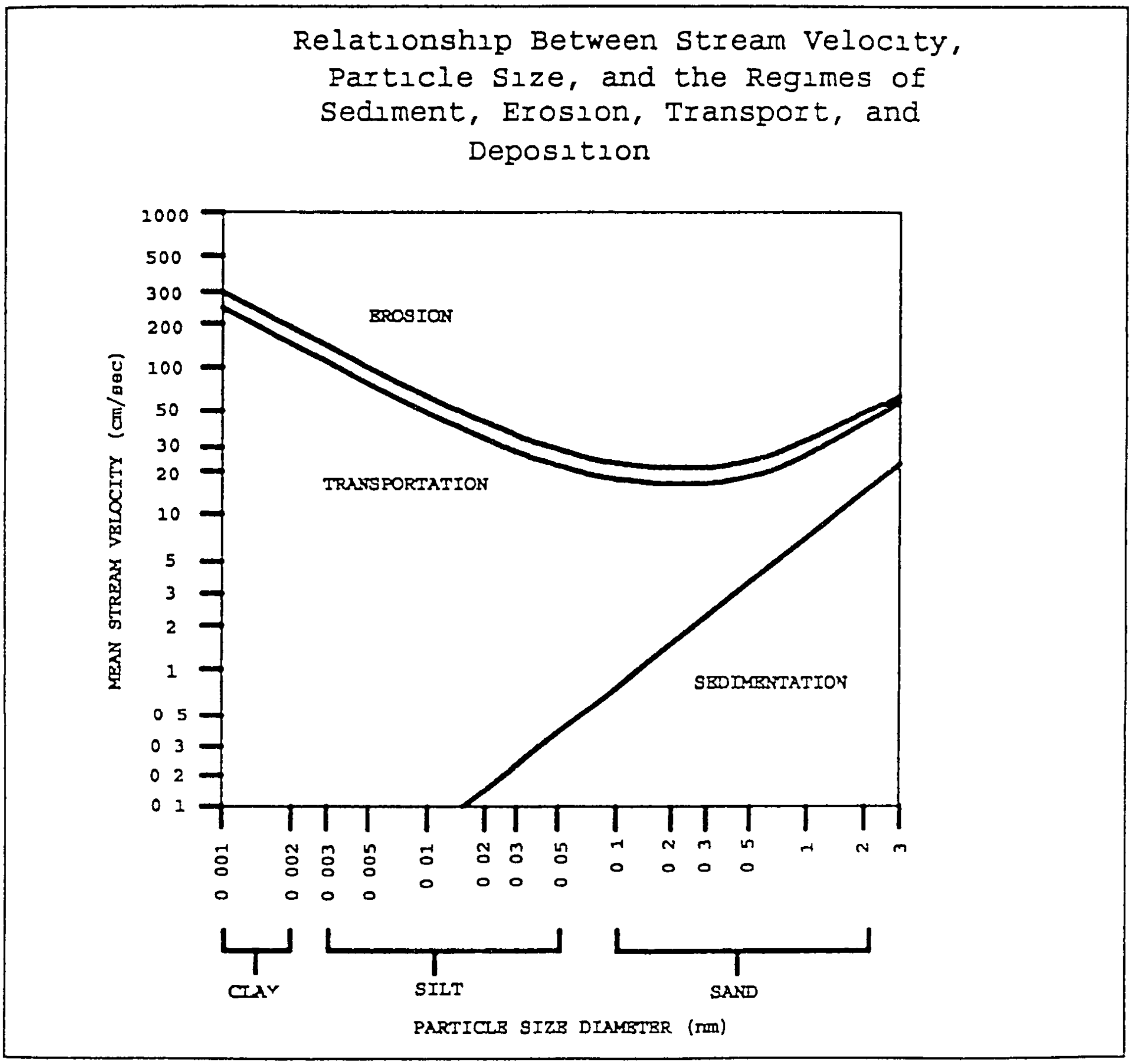


Figure 3.1 Sediment transport regimes (Graft, 1971)

on the benthic surface and the suspended sediment size and cohesiveness. Likewise, the scour velocity depends upon the shear stress, the bed sediment size and cohesiveness, and the state of consolidation of surficial benthic deposits. Figure 3.1 is offered as initial guidance in specifying initial deposition and scour velocities. For example, (coarse silt of 0.05 mm diameter may settle at 100 to 200 m/day, but should not deposit where mean stream velocity is above 0.5 cm/sec. Where mean velocity rises above 30 cm/sec, erosion is expected, and nonzero scour velocities should be specified. For fine silt of 0.005 mm diameter settling at 1 to 2 m/day,) deposition is not expected even under quiescent conditions. Nonzero scour velocities should be specified where mean velocity is above 2 m/sec. Site specific calibration is necessary to refine the initial estimates.

Sediment Loading

Sediment loading derives primarily from watershed erosion and bank erosion. These can be measured or estimated by several techniques and input into each segment as a point source load. For some problems, long term average sediment loads can be calculated using the Universal Soil Loss Equation (Wischmeier and Smith, 1978). A useful treatment of this process is given by Mill et al. (1985). This technique works poorly for short term or inherently dynamic problems because much of the sediment loading occurs during a few extreme storm or snow melt events. If available, suspended sediment data at local gaging stations can be extrapolated to provide areawide loading estimates. Alternatively, daily runoff loads can be simulated with a watershed model and read in directly from an appropriately formatted nonpoint source loading file.

The Sediment Bed

The bed sediment plays an important role in the transport and fate of water quality constituents. Sediment-sorbed pollutants may be buried in the bed by deposition and sedimentation, or they may be released to the water column by scour. In WASP5 the movement of sediment in the bed is governed by one of two options. ①In the first option, bed segment volumes remain constant and sediment concentrations vary in response to deposition and scour. No compaction or erosion of the segment volume is allowed to occur. ②In the second option, the bed segment volume is compacted or eroded as sediment is deposited or scoured. Sediment concentration in the bed remains constant. In both options chemical may be transported through the bed by pore water flow and dispersion.

The Constant Bed Volume Option--The first bed option, referred to as the constant volume option, allows the sediment concentration of the bed to change according to the net flux of sediment. Bed segments are located in reference to the rising or falling bed surface. The rate at which the bed rises or falls is represented by a sedimentation velocity, input in flow fields 3, 4, and 5 for each sediment size fraction. Sediment in the bed is added through deposition and lost through scour and sedimentation.

Assuming the depth of the bed remains constant and neglecting dispersive mixing, the mass balance of sediment in a stationary upper bed is given by

$$d_i \frac{\partial S_i}{\partial t} = w_D S_j - (w_R + w_S) S_i \qquad 3.4$$

where

w_s = sedimentation velocity of the upper bed, m/day

S_i = sediment concentration in the upper bed, g/m^3

S_j = sediment concentration in the water, g/m^3

d_i = depth of the upper bed, m

For a lower bed layer

$$d_k \frac{\partial S_k}{\partial t} = w_S S_i - w_{Sk} S_k \qquad 3.5$$

where

S_k = sediment concentration in the lower bed, g/m^3

w_{sk} = sedimentation velocity of the lower bed, m/day

d_k = depth of the lower bed, m

In most applications the sediment concentration of the bed will be nearly constant over time. In this case the mass derivative $\partial S/\partial t$ will be zero. The resulting mass balance in the upper bed is

$$w_D S_j = (w_R + w_S)\ S_i \qquad 3.6$$

In the lower bed,

$$w_s S_i = w_{sk} S_k \qquad 3\ 7$$

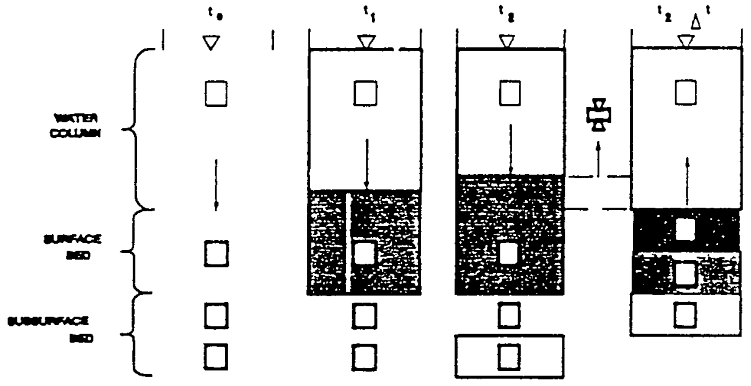
It should be noted that under the constant volume option WASP5 does not require a balance of sediment fluxes into and out of a bed segment The user should, therefore, take care that deposition, scour and sedimentation velocities reflect the intended mass flux of sediment in the bed

The constant volume option also has a provision for a movable upper bed layer This layer is modeled by specifying a total advective flow rate (flow field one) between upper bed segments Thus, when a flow rate Q_j is specified from upper bed segment j to upper bed segment i, the sediment, pore water, and chemical in j are transported to i To maintain a mass balance in segment i a similar flow rate should be specified out of i This option allows for the lateral transport of sediment across the upper bed, and can be used to represent bed load transport

The Variable Bed Volume Option--The second bed volume option, referred to as the variable bed volume option, allows bed volumes to change in response to deposition and scour Two types of bed layers are assumed an upper uncompacted layer and one or more lower compacted layers When deposition exceeds scour, the upper layer increases in volume as the surface of the bed rises After a period of time the added volume of upper bed compresses and becomes part of the lower bed When scour exceeds deposition, the volume of the upper layer decreases as the surface of the bed drops When the upper layer erodes completely, the next layer of bed is exposed to scour

In locations where sediment deposition exceeds scour (Figure 3 2), bed compaction is triggered by a sedimentation time step This sedimentation time step is input by the user and will generally be much larger than the simulation time step As sediment and sorbed chemical settle from the water column the top bed segment increases in volume sediment mass and chemical mass Sediment concentrations remain constant The volume of the upper bed continues to increase until the end of the sedimentation time step At this time the volume of the upper bed that has been added by net deposition is compressed to the density of the lower bed Since the porosity of the uncompressed bed is greater than the porosity of the compressed bed pore water and dissolved chemical are squeezed into the water column

During compression the lower bed segments rise to include the compressed portion of the upper bed The volumes and sediment concentrations of these lower bed segments remain constant A portion of the bottom bed segment is buried out of



	Time t_0			Time t_2			Time $t_2\ \Delta t$		
Segment	Depth	Density	Conc.	Depth	Density	Conc.	Depth	Density	Conc.
1	d_1	1.0	$C_1(0)$	$d_1\ d_2(0)$	1.0	$C_1(0)$	$d_1\ d_2(0)$	1.0	$C_1(0)$
2	d_2	ρ_2	0.0	$d_2(0) - d_3\frac{\rho_3}{\rho_4}$	ρ_2	$C_2(0)$	d_2	ρ_2	$C_3(0)$
3	d_3	ρ_3	0.0	d_3	ρ_3	0.0	d_3	ρ_3	$C_2(0)\frac{\rho_3}{\rho_4}$
4	d_4	ρ_4	$C_4(0)$	d_4	ρ_4	$C_4(0)$	d_4	ρ_4	0.0

Compaction: SVOL Compacted = Vol (3) $\left[\frac{\rho_3}{\rho_4}\ 1\right]$

Pore water volume SVOL squeezed

Figure 3 2 WASP4 sediment burial (variable volume option)

the network, however, as bed segments rise in response to sedimentation Thus, chemical mass in the lower bed is added through compression of the upper bed and lost through sediment burial

After compression, the top bed segment returns to its original predeposition volume Sediment and chemical concentrations in the upper bed are not changed by compaction In the lower beds segment volumes and sediment concentrations are unchanged Chemical mass from the compacted portion of the bed is added to the lower bed, and chemical mass in the bottom bed segment is buried out of the model network

Over several sedimentation time steps the density and volume of the upper bed segment remain constant, so that

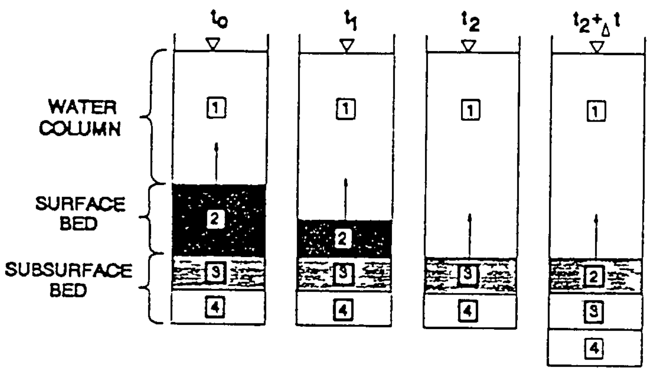
$$S_i \frac{\partial V_i}{\partial t} = A_{ij} w_D S_j - A_{ij} (w_R + w_B) S_i = 0 \qquad 3\ 8$$

and

$$w_B = (w_D S_j - w_E S_i)/S_i \tag{3 9}$$

For a lower bed layer, volumes are held constant along with density To maintain mass balance, the average sedimentation velocity is, effectively

$$w_{Bk} = w_B S_i/S_k \tag{3 10}$$



	Time - t_0			Time - t_2			Time - $t_2 + \Delta t$		
Segment	Depth	Density	Conc.	Depth	Density	Conc.	Depth	Density	Conc.
1	d_1	1 0	0.0	$d_1 + d_2(0)$	1 0	$C_1(2)$	$d_1 + d_2(0)$	1 0	1
2	d_2	ρ_2	$C_2(0)$	0	ρ_2	$C_2(0)$	d_2	ρ_2	$C_3(2)$
3	d_3	ρ_3	$C_3(0)$	d_3	ρ_3	$C_3(0)$	d_3	ρ_3	$C_4(2)$
4	d_4	ρ_4	$C_4(0)$	d_4	ρ_4	$C_4(0)$	d_4	ρ_4	0 0

Figure 3 3 WASP sediment erosion (variable volume option)

For locations where sediment scour exceeds deposition WASP responds as in Figure 3 3 As sediment and sorbed chemical erode from the bed the top bed segment decreases in volume depth chemical mass, and sediment mass Its density remains constant When the sediment mass in the top bed layer equals zero then segment renumbering is triggered All the properties of the remaining bed segments, including chemical concentration remain unaffected by renumbering The new top bed segment for example, has the same depth, volume, sediment and chemical concentration as the old second bed segment A new bottom bed segment is created with the same physical properties as the other bed segments Its chemical concentration, however is zero Renumbering and creation of a new bottom segment completes the WASP5 erosion cycle (or time step)

As a consequence of the way the variable bed volume option treats sedimentation, certain constraints are imposed on the bed segment properties defined in the input data set The density (or sediment concentration) of a top bed segment must be less than or equal to the density of the lower bed segments within a vertical stack Since the compaction routine implicitly handles sedimentation no sedimentation velocities to lower beds may be specified in the sediment transport fields Finally, the user must simulate sediment as a state variable in order to use this option Sediment is a state variable in the toxics program, but not the eutrophication program

3 2 MODEL IMPLEMENTATION

Introduction

To simulate sediment transport with WASP5 use the preprocessor or a text editor to create a TOXI5 input file Simple datasets are provided for use as templates to edit and adapt The model input dataset and the input parameters will be similar to those for the conservative tracer model as described in Chapter 2 To those basic parameters, the user will add benthic segments and solids transport rates During the simulation, solids variables will be transported both by the water column advection and dispersion rates and by these solids transport rates

In WASP5 solids transport rates in the water column and the bed are input via up to three solids transport fields These fields describe the settling deposition, scour, and sedimentation flows of three kinds of solids The transport of particulate chemicals or the particulate fraction of simulated chemicals follows the solids flows The user must specify the dissolved fraction (i e 0 0) and the solids transport field for each simulated solid under initial conditions To simulate total solids solids 1 must be used

Model Input Parameters

This section summarizes the input parameters that must be specified in order to solve the sediment balance equations in TOXI5 Input parameters are prepared for WASP5 in four major sections of the preprocessor -- environment, transport boundaries, and transformation Basic model parameters are described in Chapter 2 and will not be repeated here

Environment Parameters

These parameters define the basic model identity, including the segmentation, and control the simulation

Systems-- To simulate total solids only, select simulate" for Solids 1 and bypass" for the other five systems To simulate two solids types, select "simulate" for both Solids 1 and Solids 2 To simulate three solids types, select 'simulate" for all three The chemical systems can be simulated or bypassed (Group A Record 4, NOSYS, Record 9, SYSBY)

Bed Volume Option-- The user must determine whether bed volumes are to be held constant or allowed to vary Volumes may be held constant by specifying 0 in which case sediment concentrations and porosities in the bed segments will vary Alternatively, sediment concentrations and porosities may be held constant by specifying 1 in which case surficial bed segment volumes will vary (Group C, Record 1 IBEDV)

Bed Time Step-- While mass transport calculations are repeated every model time step, certain benthic calculations are repeated only at this benthic time step in days If the constant bed volume option is chosen, sediment concentrations are updated every model time step, but porosities are recalculated every benthic time step If the variable bed volume is chosen upper benthic segment volumes are updated every time step, with compaction occurring every benthic time step (Group C Record 1 TDINTS)

Transport Parameters

Number of Flow Fields-- To simulate total solids the user should select solids 1 flow under advection To simulate three sediment types, the user should select solids 1 flow solids 2 flow, and solids 3 flow In addition, the user should select water column flow (Group D, Record 1, NFIELD)

Sediment Transport Velocities, m/sec-- Time variable settling, deposition, scour, and sedimentation velocities can be specified for each type of solid If the units conversion factor is set to 1 157e-5, then these velocities are input in units of m/day These velocities are multiplied internally by cross-sectional areas and treated as flows that carry solids and sorbed chemical between segments Settling velocities are important components of suspended sediment transport in the water column Scour and deposition velocities determine the transfer of solids and sorbed chemical between the water column and the sediment bed Sedimentation velocities represent the rate at which the bed is rising in response to net deposition (Group D, Record 6 QT)

Cross-Sectional Areas, m^2-- The interfacial surface area must be specified for adjoining segments where sediment transport occurs These surface areas are multiplied internally by sediment transport velocities to obtain sediment transport flows (Group D, Record 4, BQ)

Boundary Parameters

This group of parameters includes boundary concentrations, waste loads, and initial conditions Boundary concentrations must be specified for any segment receiving flow inputs, outputs, or exchanges Initial conditions includes not only initial concentrations, but also the density and solids transport field for each solid, and the dissolved fraction in each segment

Boundary Concentrations, mg/L-- At each segment boundary time variable concentrations must be specified for total solids or for each solids type simulated A boundary segment is characterized by water exchanges from outside the network including tributary inflows, downstream outflows, and open water dispersive exchanges (Group E Record 4, BCT)

Waste Loads, kg/day-- For each point source discharge, time variable sediment loads can be specified for total solids or for each solids type simulated These loads can represent municipal and industrial wastewater discharges, or urban and agricultural runoff (Group F 1 Record 4 WKT)

Solids Transport Field-- The transport field associated with total solids or each solids type must be specified under initial conditions (Group J, Record 1, IFIELD)

Solid Density, g/cm^3-- The average density of the total sediment, or the density of each solids type must be specified This information is used to compute the porosity of benthic segments Porosity is a function of sediment concentration and the density of each solids type (Group J, Record 1, DSED)

Initial Concentrations, mg/L-- Concentrations of total sediment or of each solids type in each segment must be specified for the time at which the simulation begins If the variable benthic volume option is used, the benthic sediment concentrations specified here will remain constant for the entire simulation (Group J, Record 2, C)

Dissolved Fraction-- The dissolved fraction of each solid in each segment should be set to 0 (Group J Record 2, DISSF)

Transformation Parameters

This group of parameters includes spatially variable parameters constants, and kinetic time functions for the water quality constituents being simulated None are necessary for sediment transport

Data Group Descriptions

An input dataset to simulate three sediment types in a river is given with the model software A comprehensive listing of the WASP5 data groups, records, and variables is given in Part B of this documentation

CHAPTER 4

DISSOLVED OXYGEN

4 1 MODEL DESCRIPTION

Introduction

Dissolved oxygen (DO) is one of the most important variables in water quality analysis Low concentrations directly affect fish and alter a healthy ecological balance Because DO is affected by many other water quality parameters, it is a sensitive indicator of the health of the aquatic system

DO has been modeled for over 70 years The basic steady-state equations were developed and used by Streeter and Phelps (1923) Subsequent development and applications have added terms to their basic equation and provided for time-variable analysis The equations implemented here are fairly standard As explained below, the user may implement some or all of the processes that are described with terms in these equations

Overview of WASP5 Dissolved Oxygen

Dissolved oxygen and associated variables are simulated using the EUTRO5 program Several physical-chemical processes can affect the transport and interaction among the nutrients phytoplankton carbonaceous material and dissolved oxygen in the aquatic environment Figure 4 1 presents the principal kinetic interactions for the nutrient cycles and dissolved oxygen

EUTRO5 can be operated by the user at various levels of complexity to simulate some or all of these variables and interactions To simulate only carbonaceous biochemical oxygen demand (BOD) and DO, for example, the user may bypass calculations for the nitrogen phosphorus and phytoplankton variables Simulations may incorporate ① carbonaceous biochemical oxygen demand (CBOD) and either ② ammonia (NH3) or nitrogenous biochemical oxygen demand (NBOD) expressed as ammonia ③ Sediment oxygen demand may be specified, as well as photosynthesis and respiration rates

Four levels of complexity are identified and documented at the end of this section (1) Streeter-Phelps (2) modified Streeter-Phelps (3) full linear DO balance and (4) nonlinear DO balance The actual simulation of phytoplankton is described in Chapter 5

Dissolved Oxygen Processes

TABLE ~~1 4 7~~ 4 1 CBOD AND DO REACTION TERMS

escription	Notation	Value from Potomac Estuary Model	Units
oxygen to carbon ratio	a_{OC}	32/12	mg O_2/mg C
ratio of the ultimate to 5 day carbonaceous biochemical oxygen demand	BOD_{U5}	1 85	none
deoxygenation rate @ 20 C	k_d	0 21 0 16	day^{-1}
temperature coefficient	θ_d	1 047	none
half saturation constant for oxygen limitation	K_{BOD}	0 5	mg O_2/L
oxygen to nitrogen ratio	a_{ON}	32/14	mg O_2/mg N
oxygen to carbon ratio for nitrate uptake	a_{NO_3C}	$(48/14)a_{NC}$	mg O_2/mg C
reaeration rate @ 20 C	k_a k_2	cf Eq 1 4 32 1 4 34	day ^{1}
temperature coefficient	θ_a θ	1 028	none
dissolved oxygen saturation	DO_{sat}	cf Eq 1 4 37	mg O_2/L
fraction dissolved CBOD	f_{D5}	0 5	none
organic matter settling velocity	v_{s3}		m/day

Five EUTRO5 state variables can participate directly in the DO balance phytoplankton carbon, ammonia, nitrate, carbonaceous biochemical oxygen demand, and dissolved oxygen The reduction of dissolved oxygen is a consequence of the aerobic respiratory processes in the water column and the anaerobic processes in the underlying sediments Because both these sets of processes can contribute significantly, it is necessary to formulate their kinetics explicitly

The methodology for the analysis of dissolved oxygen dynamics in natural waters, particularly in streams, rivers and estuaries is reasonably well-developed (O Connor and Thomann, 1972) The major and minor processes incorporated into EUTRO5 are discussed below The reader should refer to the kinetic equations summarized in Figure 4 2 and the reaction parameters and coefficients in Table 4 1

5. *CARBONBACEOUS BIOCHEMICAL OXYGEN DEMAND*

$$\frac{\partial C_5}{\partial t} = \underbrace{a_{oc} K_{1D} C_4}_{\textit{death}} - \underbrace{k_D \Theta_D^{(T-20)} \left(\frac{C_6}{K_{BOD} + C_6} \right) C_5}_{\textit{oxidation}} - \underbrace{\frac{v_{S3} (1 - f_{D5})}{D} C_5}_{\textit{settling}}$$

$$- \underbrace{\frac{5}{4} \frac{32}{14} k_{2D} \Theta_{2D}^{(T-20)} \left(\frac{K_{NO3}}{K_{NO3} + C_6} \right) C_2}_{\textit{denitrification}}$$

6. *DISSOLVED OXYGEN*

$$\frac{\partial C_6}{\partial t} = \underbrace{k_2 (C_S - C_6)}_{\textit{reaeration}} - \underbrace{k_d \Theta_d^{T-20} \left(\frac{C_6}{K_{BOD} + C_6} \right) C_5}_{\textit{oxidation}} - \underbrace{\frac{64}{14} k_{12} \Theta_{12}^{T-20} \left(\frac{C_6}{K_{NIT} + C_6} \right) C_1}_{\textit{nitrification}}$$

$$- \underbrace{\frac{SOD}{D} \Theta_S^{T-20}}_{\textit{sediment demand}} + \underbrace{G_{P1} \left(\frac{32}{12} + \frac{48}{14} \frac{14}{12} (1 - P_{NH3}) \right) C_4}_{\textit{phytoplankton growth}} - \underbrace{\frac{32}{12} k_{1R} \Theta_{1R}^{T-20} C_4}_{\textit{respiration}}$$

Figure 4 2 Oxygen balance equations

Reaeration

Oxygen deficient, i e , below saturation, waters are replenished via atmospheric reaeration The reaeration rate coefficient is a function of the average water velocity depth wind, and temperature. In EUTRO5, the user may specify a single reaeration rate constant, spatially-variable reaeration rate constants, or allow the model to calculate variable reaeration rates based upon flow or wind. Calculated reaeration will follow either the flow-induced rate or the wind-induced rate, whichever is larger.

EUTRO5 calculates flow-induced reaeration based on the Covar method (Covar, 1976). This method calculates reaeration as a function of velocity and depth by one of three formulas -- Owens, Churchill, or O'Connor- Dobbins, respectively:

$$k_{qj}(20^\circ C) = 5.349\, v_j^{0.67}\, D_j^{-1.85} \qquad 4.1$$

$$k_{qj}(20^\circ C) = 5.049\, v_j^{0.97}\, D_j^{-1.67} \qquad 4.2$$

or

$$k_{qj}(20^\circ C) = 3.93\, v_j^{0.50}\, D_j^{-1.50} \qquad 4.3$$

where

k_{qj} = flow-induced reaeration rate coefficient at 20°C, day^{-1}

v_j = average water velocity in segment j, m/sec

D_j = average segment depth, m

The Owens formula is automatically selected for segments with depth less than 2 feet. For segments deeper than 2 feet, the O'Connor-Dobbins or Churchill formula is selected based on a consideration of depth and velocity. Deeper, slowly moving rivers require O'Connor-Dobbins, moderately shallow, faster moving streams require Churchill. Segment temperatures are used to adjust the flow-induced $k_{qj}(20\,^\circ C)$ by the standard formula

$$k_{aj}(T) = k_{aj}(20°C)\ \theta_a^{T-20} \tag{4 4}$$

where

T = water temperature, 蚓

$k_{aj}(T)$ = reaeration rate coefficient at ambient segment temperature, day ^{1}

θ_a = temperature coefficient, unitless

Wind-induced reaeration is determined by O'Connor (1983) This method calculates reaeration as a function of wind speed air and water temperature, and depth using one of three formulas

$$k_{wj} = \frac{86400}{100D_j}\left(\frac{D_{OW}}{\nu_W}\right)^{2/3}\left(\frac{\rho_a}{\rho_W}\right)^{1/2}\frac{\kappa^{1/3}}{\Gamma}\sqrt{C_d}\ (100\ W) \tag{4 5}$$

$$k_{wj} = \frac{86400}{100D_j}\left[(TERM1\ 100W)^{-1} + (TERM2\sqrt{100W})^{-1}\right]^{-1}$$

where

$$TERM1 = \left(\frac{D_{OW}}{\nu_W}\right)^{2/3}\left(\frac{\rho_a}{\rho_W}\right)^{1/2}\frac{\kappa^{1/3}}{\Gamma_u}\sqrt{C_d} \tag{4 6}$$

$$TERM2 = \left(\frac{D_{OW}}{\kappa z_0}\ \frac{\rho_a \nu_a}{\rho_W \nu_W}\sqrt{C_d}\right)^{1/2}$$

or

$$k_{wj} = \frac{86400}{100D_j}\left(\frac{D_{OW}}{\kappa z_e}\ \frac{\rho_a \nu_a}{\rho_W \nu_W}\sqrt{C_d}\right)^{1/2}\sqrt{100W} \tag{4 7}$$

where

k_{w} = wind-induced reaeration rate coefficient, day^{-1}

W = time-varying wind speed at 10 cm above surface, m/sec

T_a = air temperature, °C

ρ_a = density of air, a function of T_a g/cm^3

ρ_w = density of water, 1.0 g/cm^3

ν_a = viscosity of air, a function of T_a, cm^2/s

ν_w = viscosity of water, a function of T, cm^2/s

D_{ow} = diffusivity of oxygen in water a function of T cm^2/s

κ = von Karman's coefficient, 0.4

v_t = transitional shear velocity, set to 9, 10, and 10 for small, medium, and large scales, cm/s

v_c = critical shear velocity, set to 22, 11, and 11 for small, medium, and large scales, cm/s

z_e = equivalent roughness, set to 0.25, 0.35, and 0.35 for small, medium, and large scales, cm

z_0 = effective roughness, a function of z_e, Γ, C_d, v_t, ν_a, and W, cm

λ = inverse of Reynold's number, set to 10, 3, and 3 for small, medium, and large scales

Γ = nondimensional coefficient, set to 10, 6.5, and 5 for small, medium, and large scales

Γ_u = nondimensional coefficient, a function of Γ, v_c, C_d, and W

C_d = drag coefficient, a function of z_e, Γ, ν_a, κ, v, and

Equation 4.5 is used for wind speeds of up to 6 m/sec where interfacial conditions are smooth and momentum transfer is dominated by viscous forces. Equation 4.7 is used for wind speeds over 20 m/sec where interfacial conditions are rough and momentum transfer is dominated by turbulent eddies. Equation 4.6 is used for wind speeds between 6 and 20 m/sec and represents a transition zone in which the diffusional sublayer decays and the roughness height increases.

The user is referred to O'Connor (1983) for details on the calculation of air density, air and water viscosity, the drag coefficient the effective roughness, and Γ_L Small scale represents laboratory conditions Large scale represents open ocean conditions Medium scale represents most lakes and reservoirs

Dissolved oxygen saturation C_s, is determined as a function of temperature, in degrees K and salinity S, in mg/L (APHA 1985)

$$\begin{aligned} \ln C_s = {} & -139\ 34 + (1\ 5757\ \ 10^{5})\, T_K^{-1} - (6\ 6423\ \ 10^{7})\, T_K^{-2} \\ & + (1\ 2438\ \ 10^{10})\, T_K^{-3} - (8\ 6219\ \ 10^{11})\, T_K^{-4} \\ & - 0\ 5535\, S(0\ 031929 - 19\ 428\, T_K^{-1} + 3867\ 3\, T_K^{-2}) \end{aligned} \qquad 4\ 8$$

Carbonaceous Oxidation

The long history of applications have focused primarily on the use of BOD as the measure of the quantity of oxygen demanding material and its rate of oxidation as the controlling kinetic reaction This has proven to be appropriate for waters receiving a heterogeneous combination of organic wastes of municipal and industrial origin since an aggregate measure of their potential effect is a great simplification that reduces a complex problem to one of tractable dimensions

The oxidation of carbonaceous material is the classical BOD reaction Internally the model uses ultimate carbonaceous biochemical oxygen demand CBOD as the indicator of equivalent oxygen demand for the carbonaceous material A principal source of CBOD other than man-made sources and natural runoff is detrital phytoplankton carbon produced as a result of algal death The primary loss mechanism associated with CBOD is oxidation

$$C_xH_yO_z \rightarrow CO_2 + H_2O \qquad 4\ 9$$

The kinetic expression for carbonaceous oxidation in EUTRO5 contains three terms -- a first order rate constant a temperature correction term and a low DO correction term The first two terms are standard The third term represents the decline of the aerobic oxidation rate as DO levels approach 0 The user may specify the half-saturation constant K_{BOD}, which represents the DO level at which the oxidation rate is reduced by half The default value is zero which allows this reaction to proceed fully even under anaerobic conditions

Direct comparisons between observed BOD_5 data and model output cannot be made using the internal CBOD computed by EUTRO5 since field measurements may be tainted by algal respiration and the decay of algal carbon Therefore a correction must be made to the internally computed model CBOD so that a valid comparison to the field measurement may be made This results in a new variable known as the bottle BOD_5 which is computed via equation 4 10

$$\begin{aligned} Bottle\ BOD_5 = {} & C_5\,(1 - e^{-5k_{dbot}}) + \frac{64}{14}C_1\,(1 - e^{-5k_{nbot}}) \\ & + a_{oc}C_4\,(1 - e^{-5k_{1R}}) \end{aligned} \qquad 4\ 10$$

where

C_5 = the internally computed CBOD, mg/L

C_1 = the internally computed NH_3, mg/L

C_4 = the phytoplankton biomass in carbon units, mg/L

a_{oc} = the oxygen to carbon ratio, 32/12 mg O_2/mg C

k_{dbot} = the laboratory 'bottle' deoxygenation rate constant, day^{-1}

k_{nbot} = the laboratory 'bottle' nitrification rate constant, day^{-1}

k_{1R} = the algal respiration rate constant at 20°C day $^{-1}$

Equation 4 10 can provide a low estimate of the observed bottle BOD because it does not include a correction for the decay of detrital algal carbon which in turn depends upon the number of non-viable phytoplankton Please note that laboratory 'bottle' CBOD and nitrification rates are used here, as specified by the user The default laboratory rate constant for nitrification is 0, reflecting the use of a nitrifying inhibitor

Nitrification

Additional significant losses of oxygen can occur as a result of nitrification

$$NH_3^+ + 2O_2 \rightarrow NO_3 + H_20 + H^+ \qquad 4\ 11$$

Thus for every mg of ammonia nitrogen oxidized, 2 (32/14) mg of oxygen are consumed

The kinetic expression for nitrification in EUTRO5 contains three terms -- a first order rate constant, a temperature correction term, and a low DO correction term The first two terms are standard The third term represents the decline of the nitrification rate as DO levels approach 0 The user may specify the half-saturation constant K_{NIT}, which represents the DO level at which the nitrification rate is reduced by half The default value is zero, which allows this reaction to proceed fully even under anaerobic conditions

Denitrification

Under low DO conditions, the denitrification reaction provides a sink for CBOD

$$5CH_20 + 5H_2O + 4NO_3 + 4H^+ \rightarrow 5CO_2 + 2N_2 + 12H_2O \qquad 4\ 12$$

Thus for each mg of nitrate nitrogen reduced 5/4 (12/14) mg of carbon are consumed which reduces CBOD by 5/4 (12/14) (32/12) mg Denitrification is not a significant loss in the water column, but can be important when simulating anaerobic benthic conditions

The kinetic expression for denitrification in EUTRO5 contains three terms -- a first order rate constant (with appropriate stoichiometric ratios), a temperature correction term and a DO correction term The first two terms are standard The third term represents the decline of the denitrification rate as DO levels rise above 0 The user may specify the half-saturation constant K_{NO3} which represents the DO level at which the denitrification rate is reduced by half The default value is zero, which prevents this reaction at all DO levels

Settling

Under quiescent flow conditions, the particulate fraction of CBOD can settle downward through the water column and deposit on the bottom. In water bodies, this can reduce carbonaceous deoxygenation in the water column significantly. The deposition of CBOD and phytoplankton, however, can fuel sediment oxygen demand in the benthic sediment. Under high flow conditions particulate CBOD from the bed can be resuspended.

The kinetic expression for settling in EUTRO5 is driven by the user-specified particulate settling velocity v_{s3} and the CBOD particulate fraction $(1 - f_{D5})$, where f_{D5} is the dissolved fraction. Settling velocities that vary with time and segment can be input as part of the advective transport field. Resuspension can also be input using a separate velocity time function. Segment-variable dissolved fractions are input with initial conditions.

Phytoplankton Growth

A byproduct of photosynthetic carbon fixation is the production of dissolved oxygen. The rate of oxygen production (and nutrient uptake) is proportional to the growth rate of the phytoplankton since its stoichiometry is fixed. Thus, for each mg of phytoplankton carbon produced by growth, 32/12 mg of O_2 are produced. An additional source of oxygen from phytoplankton growth occurs when the available ammonia nutrient source is exhausted and the phytoplankton begin to utilize the available nitrate. For nitrate uptake the initial step is a reduction to ammonia which produces oxygen:

$$2NO_3 \rightarrow 2NH_3 + 3O_2 \qquad 4.13$$

Thus, for each mg of phytoplankton carbon produced by growth using nitrate, a_{NC} mg of phytoplankton nitrogen are reduced, and (48/14) a_{NC} mg of O_2 are produced.

Phytoplankton Respiration

Oxygen is diminished in the water column as a result of phytoplankton respiration, which is basically the reverse process of photosynthesis:

$$C_4 + O_2 \rightarrow CO_2 \qquad 4.14$$

where C_4 is phytoplankton carbon in mg/L Thus for every mg of phytoplankton carbon consumed by respiration, 32/12 mg of oxygen are also consumed

Phytoplankton Death

The death of phytoplankton provides organic carbon, which can be oxidized The kinetic expression in EUTRO5 recycles phytoplankton carbon to CBOD using a first order death rate and the stoichiometric oxygen to carbon ratio 32/12

Sediment Oxygen Demand

The decomposition of organic material in benthic sediment can have profound effects on the concentrations of oxygen in the overlying waters The decomposition of organic material results in the exertion of an oxygen demand at the sediment-water interface As a result, the areal fluxes from the sediment can be substantial oxygen sinks to the overlying water column

EUTRO5 provides two options for oxygen fluxes descriptive input and predictive calculations The first option is used for networks composed of water column segments only The kinetic equation is given in Figure 4 2 Observed sediment oxygen demand fluxes must be specified for water segments in contact with the benthic layer Seasonal changes in water temperature can affect SOD through the temperature coefficient

The calculational framework incorporated for benthic-water column exchange draws principally from a study of Lake Erie, which incorporated sediment-water column interactions performed by Di Toro and Connolly (1980) For a single benthic layer with thickness, Dj the CBOD and DO mass balance equations are summarized in Figure 4 3 The equivalent SOD generated for the overlying water column segment is also given Subscripts 'j and i refer to a benthic segment and the overlying water column segment, respectively

WASP5 allows a more detailed parameterization of settling into the benthos that includes not only a downward settling velocity but an upward resuspension velocity as well In this context then the net particulate flux to the sediment is due to the difference between the downward settling flux and the upward resuspension flux

One of the first decisions to be made regarding the benthic layer is to determine its depth Two factors influence this decision The first is to adequately reflect the thickness of the active layer, the depth to which the sediment is influenced by exchange with the overlying water column Secondly one wishes the model to reflect a reasonable time history or memory of the sediment layer Too thin a layer and the benthos will remember

5. CARBONACEOUS BIOCHEMICAL OXYGEN DEMAND

$$\frac{\partial C_{5j}}{\partial t} = \underset{\text{decomposition}}{a_{OC} k_{PZD} \Theta_{PZD}^{T-20} C_{4j}} - \underset{\text{oxidation}}{k_{DS} \Theta_{DS}^{T-20} C_{5j}} - \underset{\text{denitrification}}{\frac{5}{4} \frac{32}{14} k_{2D} \Theta_{2D}^{T-20} C_{2j}}$$

$$+ \underset{\text{settling}}{\frac{v_{B3}}{D_j} (1 - f_{D5i})\, C_{5i}} - \underset{\text{resuspension}}{\frac{v_{R3}}{D_j} (1 - f_{D5j})\, C_{5j}} + \underset{\text{diffusion}}{\frac{E_{DIF}}{D_j^2} (C_{5i} f_{D5i} - C_{5j} f_{D5j})}$$

6. DISSOLVED OXYGEN

$$\frac{\partial C_{6j}}{\partial t} = - \underset{\text{oxidation}}{k_{DS} \Theta_{DS}^{T-20}} + \underset{\text{diffusion}}{\frac{E_{DIF}}{D_j^2} (C_{6i} - C_{6j})}$$

SEDIMENT OXYGEN DEMAND (g/m²-day)

$$SOD = \frac{E_{DIF}}{D_j} (C_{6i} - C_{6j})$$

(*for benthic segment j, water segment i*)

Figure 3 Benthic layer oxygen balance equations or be influenced by deposition of material that would have occurred only within the last year or two of the period being analyzed too thick a layer and the model will average too long a history, not reflecting substantial reductions resulting from reduced discharges from sewage treatment plants The choice of sediment thickness is further complicated by spatially variable sedimentation rates The benthic layer depths, together with the assigned sedimentation velocities, provide for a multi-year detention time or 'memory', providing a reasonable approximation of the active layer in light of the observed pore water gradients

The decomposition reactions that drive the component mass balance equations are the anaerobic decomposition of the phytoplankton carbon, and the anaerobic breakdown of the benthic organic carbon Both reactions are sinks of oxygen and rapidly drive its concentration negative, indicating that the sediment is reduced rather than oxidized The negative concentrations computed can be considered the oxygen equivalents of the reduced end products produced by the chains of redox reactions occurring in the sediment

Because the calculated concentration of oxygen is positive in the overlying water, it is assumed that the reduced carbon species (negative oxygen equivalents) that are transported across the benthic water interface combine with the available oxygen and are oxidized to CO_2 and H_2O with a consequent reduction of oxygen in the overlying water column

Figure 4 3 and Table 4 2 summarize the benthic CBOD and DO reactions and parameters Illustrative parameter values from an early Potomac Estuary modeling study are provided

4 2 MODEL IMPLEMENTATION

To simulate dissolved oxygen with WASP5 use the preprocessor to create a EUTRO5 input dataset For the portions of the dataset describing environment, transport, and boundaries EUTRO5 model input will be similar to that for the conservative tracer model as described in Chapter 2 To those basic parameters, the user will add combinations of transformation parameters and perhaps solids transport rates

EUTRO5 kinetics can be implemented using some or all of the processes and kinetic terms described above to analyze dissolved oxygen problems For convenience, four levels of complexity are identified here (1) Streeter-Phelps, (2) modified Streeter-

TABLE 4 2 Benthic Layer CBOD and DO Reaction Terms

Description	Notation	Value	Units
Organic carbon (as CBOD) decomposition rate	k_{DS}	0 0004	day^{1}
Temperature coefficient	θ_{DS}	1 08	none
Denitrification rate	k_{2D}		day^{1}
Temperature coefficient	θ_{2D}		none
Phytoplankton decomposition rate	k_{PzD}		day$_{1}$
Temperature coefficient	θ_{PzD}		none
Diffusive exchange coefficient	E_{DIF}	2 0 x 10^{4}	m^2/day
Benthic layer depth	D_j	0 2-0 7	m
Benthic layer	j		
Water column	i		

Phelps (3) full linear DO balance, and (4) nonlinear DO balance Please note that the discrete levels of simulation identified here are among a continuum of levels that the user could implement

The four implementation levels are described briefly below along with the input parameters required to solve the DO balance equations in EUTRO5 Input parameters are prepared for WASP5 in four major sections of the preprocessor -- environment transport boundaries, and transformation Basic model parameters are described in Chapter 2 and will not be repeated here Six of the eight EUTRO5 state variables that can participate in DO balance simulations, with abbreviations used in this text, are listed in Table 4 3

Streeter-Phelps

The simplest dissolved oxygen balance solves the Streeter-Phelps BOD-DO equations in a slightly modified form

$$S_{k5} = -k_d \theta_d^{T-20} C_5 - \frac{v_{B3}}{D} (1 - f_{D5}) C_5 \qquad 4\ 15$$

Table 4 3 Summary of EUTRO5 Variables Used in DO Balance

	Variable	Notation	Concentration	Units
1	Ammonia Nitrogen	NH3	C_1	mg N/L
2	Nitrate Nitrogen	NO3	C_2	mg N/L
4	Phytoplankton Carbon	PHYT	C	mg C/L
5	Carbonaceous BOD	CBOD	C_5	mg O_2/L
6	Dissolved Oxygen	DO	C_6	mg O_2/L
6	Organic Nitrogen	ON	C_7	mg N/L

$$S_{k6} = +k_2 \theta_2^{T-20} (C_s - C_6) - k_d \theta_d^{T-20} C_5 - \frac{SOD}{D} \tag{4 16}$$

where S_{ki} is the source/sink term for variable i" in a segment, in mg/L-day Kinetic rate constants and coefficients are as defined in Table 4 1 except that C_5 is interpreted as total (not just carbonaceous) biochemical oxygen demand, BOD These equations are usually applied in well-defined low flow design conditions

Environment Parameters

These parameters define the basic model identity, including the segmentation and control the simulation

Systems-- Select "simulate for CBOD and DO and 'bypass for the other six systems For this implementation the CBOD system is used to represent total ultimate BOD (Group A Record 4 NOSYS Record 9, SYSBY)

Segments-- Water column segments should be defined in the standard fashion If BOD settling is to be simulated the user should add a single benthic segment underlying all water column segments This benthic segment will merely act as a convenient sink for settling BOD Model calculations within this benthic segment should be ignored (Group A, Record 4 NOSEG, Group C, Record 3, ISEG, IBOTSG, ITYPE, BVOL, DMULT)

Transport Parameters

This group of parameters defines the advective and dispersive transport of simulated model variables

Number of Flow Fields-- To simulate settling the user should select solids 1 flow under advection The user should also select water column flow (Group D, Record 1, NFIELD)

Particulate Transport, m^3/sec-- Time variable settling and resuspension rates for particulate BOD can be input using the Solids 1 continuity array BQ and the time function QT For each solids flow field, cross-sectional exchange areas (m^2) for adjacent segment pairs are input using the spatially-variable BQ Time-variable settling velocities can be specified as a series of velocities, in m/sec versus time If the units conversion factor is set to 1 157e-5 then these velocities are input in units of m/day These velocities are multiplied internally by cross-sectional areas and treated as flows that carry particulate organic matter out of the water column (Group D Record 4, BQ JQ, IQ, Record 6, QT, TQ)

Boundary Parameters

This group of parameters includes boundary concentrations waste loads and initial conditions Boundary concentrations must be specified for any segment receiving flow inputs, outputs, or exchanges Initial conditions include not only initial concentrations, but also the density and solids transport field for each solid, and the dissolved fraction in each segment

Boundary Concentrations, mg/L-- At each segment boundary time variable concentrations must be specified for BOD and DO A boundary segment is characterized by water exchanges from outside the network including tributary inflows downstream outflows and open water dispersive exchanges (Group E Record 4 BCT)

Waste Loads, kg/day-- For each point source discharge, time variable BOD and DO loads can be specified These loads can represent municipal and industrial wastewater discharges, or urban and agricultural runoff (Group F 1, Record 4 WKT)

Solids Transport Field-- The transport field associated with particulate BOD settling must be specified under initial conditions Field 3 is recommended (Group J Record 1, IFIELD)

Solid Density, g/cm^3-- A value of 0 can be entered for the nominal density of BOD and DO This information is not used in EUTRO5 (Group J, Record 1, DSED)

Initial Concentrations, mg/L-- Concentrations of BOD and DO in each segment must be specified for the time at which the simulation begins Concentrations of zero for nonsimulated variables -- NH3 NO3, PO4, PHYT, ON, and OP -- will be entered by the preprocessor (Group J, Record 2, C)

Dissolved Fraction-- The dissolved fraction of BOD and DO in each segment must be specified Values for DO should be 1 0 Only the particulate fraction of BOD will be subject to settling (Group J, Record 2, DISSF)

Transformation Parameters

This group of parameters includes spatially variable parameters, constants, and kinetic time functions for the water quality constituents being simulated Parameter values are entered for each segment Specified values for constants apply over the entire network for the whole simulation Kinetic time functions are composed of a series of values versus time, in days

Water Temperature, °C-- Segment variable water temperatures can be specified using the parameter TMPSG (parameter TMPFN and time functions TEMP(1-4) should be omitted) Temperatures will remain constant in time (Group G Record 4, PARAM(I,3))

Sediment Oxygen Demand, g/m^2-day-- Segment variable sediment oxygen demand fluxes can be specified using the parameter SOD1D Values should be entered for water column segments that are in contact with the bottom of the water body (Group G, Record 4 PARAM(I,9))

BOD Deoxygenation Rate, day^{-1}-- The BOD deoxygenation rate constant and temperature coefficient can be specified using constants KDC and KDT, respectively (Group H, Record 4, CONST(72) CONST(73))

Reaeration Rate, day^{-1}-- There are three options for specifying reaeration rate constants in EUTRO5 In the first option, a single reaeration rate constant can be specified using constant K2 (Constant 82) An internal temperature coefficient of 1 028 is used with this option

If K2 is not entered (or is set to 0) the second option is attempted by EUTRO5 In this option, variable reaeration rate constants can be input using parameter REARSG and time function REAR The product of spatially-variable REARSG and time-variable REAR gives the segment and time specific reaeration rate constants used by EUTRO5 These reaeration values are not modified by a temperature function

The third option is invoked if neither K2 nor REARSG is entered In this option reaeration rates will be calculated from water velocity, depth, wind velocity, and water and air temperature The actual reaeration rate used by EUTRO5 will b either the flow or wind-induced value whichever is largest

For rivers, segment water velocities and depths are calculated as a function of flow using the hydraulic coefficien entered under the topic "environment" (Group C, Record 3 a b c, d) For lakes and estuaries, ambient velocities in m/sec can be input using parameter VELFN and time functions VEL(1-4) The parameter VELFN indicates which velocity function will be used b the model for each segment Values of 1 0, 2 0, 3 0, or 4 0 will call time functions VELN(1), VELN(2), VELN(3), and VELN(4), respectively Water velocities should then be entered via these time functions as a series of velocity versus time values

For open bodies of water, wind-driven reaeration can be significant The user should input ambient wind speed in m/sec and air temperature, in [illegible], using time functions WIND and AIRTMP The default values for wind speed and air temperature are 0 6 m/sec and 15 C The scale of the water body should be input using constant WTYPE Values of 1 0, 2 0, and 3 0 indicate laboratory scale, lake and reservoir scale, and open ocean scale respectively The default value is 2

For estuaries, where salinity affects DO saturation significantly salinity values in g/L can be input using parameter SAL and time function SALFN The product of spatially variable SAL and time-variable SALFN gives the segment and time specific salinity values used by EUTRO5 Average segment salinity values can be input to SAL while relative variations time, if significant can be input to SALFN

For northern climates, where ice cover can affect reaeratio during winter months, the user may input the fraction of water surface available for reaeration using time function XICECVR value of 1 0 indicates that the entire surface area is available for reaeration The time variable value of XICECVR will be multiplied by the reaeration rate constants for options 1 and 3 For option 2, it is assumed that ice cover is built into the t function REAR

WTYPE and K2 are identified in EUTRO5 as constants 1 and 82 VELFN SAL, and REARSG are identified in EUTRO5 as parameters 2 and 14, respectively WIND, VELN(1-4) SALFN AIRTMP XICECVR and REAR are identified in EUTRO5 as time functions 7 15-18, 20 21, 22, and 23 respectively (Group G Record 4, PARAM(I 1), PARAM(I,2), PARAM(I,14) Group H, Record 4 CONST(82) Group I Record 2, VALT(7 K) VALT(15-18 K) VALT(20 K) VALT(21,K), VALT(22 K), VALT(23,K))

Modified Streeter-Phelps

The modified Streeter-Phelps equations divide biochemical oxygen demand into carbonaceous and nitrogenous fractions and allow time-variable temperatures to be specified. This allows for more realistic calibration to observed data. Waste load allocations, however, are usually projected for design low-flow conditions.

$$S_{k5} = -k_d\,\theta_d^{T-20}\,C_5 - \frac{v_{B3}}{D}(1 - f_{D5})\,C_5 \tag{4.17}$$

$$S_{k1} = -k_n\,\theta_n^{T-20}\,C_1 - \frac{v_{B3}}{D}(1 - f_{D1})\,C_1 \tag{4.18}$$

$$\begin{aligned} S_{k6} = {} & +k_2\,\theta_2^{T-20}\,(C_s - C_6) - k_d\,\theta_d^{T-20}\,C_5 \\ & - \frac{64}{14}k_n\,\theta_n^{T-20}\,C_1 - \frac{SOD}{D}\,\theta_s^{T-20} \end{aligned} \tag{4.19}$$

where S_{ki} is the source/sink term for variable 'i' in a segment, in mg/L-day. Kinetic rate constants and coefficients are as defined in Table 4.1, except for the following:

C_1 = nitrogenous biochemical oxygen demand (NBOD), as expressed by TKN, mg/L (use System 1)

k_n = nitrogenous deoxygenation rate constant, day^{-1}

θ_n = temperature coefficient

f_{D1} = NBOD dissolved fraction

To implement these equations in EUTRO5, System 1 (nominally NH3) must be interpreted as nitrogenous BOD rather than ammonia. Here, NBOD is expressed by total kjeldahl nitrogen (TKN). If directly measured NBOD data are available, values should be divided by 4.57 before use in this model. Likewise, System 1 model predictions should be multiplied by 4.57 before comparison with NBOD data.

Environment Parameters

These parameters define the basic model identity, including the segmentation, and control the simulation.

Systems-- Select 'simulate' for NH3, CBOD and DO and 'bypass' for the other five systems. For this implementation, the NH3 system is used to represent nitrogenous BOD, as expressed by TKN (Group A Record 4, NOSYS, Record 9, SYSBY)

Segments-- Water column segments should be defined in the standard fashion If CBOD or NBOD settling is to be simulated the user should add a single benthic segment underlying all water column segments This benthic segment will merely act as a convenient sink for settling BOD Model calculations within this benthic segment should be ignored (Group A, Record 4 NOSEG Group C, Record 3, ISEG, IBOTSG, ITYPE, BVOL, DMULT)

Transport Parameters

This group of parameters define the advective and dispersive transport of model variables

Number of Flow Fields-- To simulate settling the user should select solids 1 flow under advection The user should also select water column flow (Group D Record 1 NFIELD)

Particulate Transport, m^3/sec-- Time variable settling and resuspension rates for particulate CBOD and NBOD can be input using the Solids 1 continuity array BQ and the time function QT For each solids flow field cross-sectional exchange areas (m^2) for adjacent segment pairs are input using the spatially-variable BQ Time-variable settling velocities can be specified as a series of velocities in m/sec versus time If the units conversion factor is set to 1 157e-5, then these velocities are input in units of m/day These velocities are multiplied internally by cross-sectional areas and treated as flows that carry particulate organic matter out of the water column (Group D, Record 4, BQ JQ IQ Record 6 QT TQ)

Boundary Parameters

This group of parameters includes boundary concentrations waste loads, and initial conditions Boundary concentrations must be specified for any segment receiving flow inputs outputs or exchanges Initial conditions include not only initial concentrations but also the density and solids transport field for each solid and the dissolved fraction in each segment

Boundary Concentrations, mg/L-- At each segment boundary time variable concentrations must be specified for CBOD NBOD and DO The NH3 system is used to represent NBOD, which is expressed as TKN A boundary segment is characterized by water exchanges from outside the network including tributary inflows downstream outflows and open water dispersive exchanges (Group E, Record 4 BCT)

Waste Loads, kg/day-- For each point source discharge time variable CBOD, NBOD, and DO loads can be specified These loads can represent municipal and industrial wastewater discharges, or urban and agricultural runoff The NH3 system is used to represent NBOD, which is expressed as TKN (Group F 1, Record 4 WKT)

Solids Transport Field-- The transport field associated with particulate CBOD and NBOD settling must be specified under initial conditions Field 3 is recommended for both (Group J, Record 1, IFIELD)

Solid Density, g/cm^3-- A value of 0 can be entered for the nominal density of CBOD, NBOD, and DO This information is not used in EUTRO5 (Group J, Record 1, DSED)

Initial Concentrations, mg/L-- Concentrations of CBOD NBOD and DO in each segment must be specified for the time at which the simulation begins The NH3 system is used to represent NBOD, which is expressed as TKN Concentrations of zero for non-simulated variables -- NO3, PO4, PHYT, ON, and OP -- will be entered by the preprocessor (Group J, Record 2, C)

Dissolved Fraction-- The dissolved fraction of CBOD, NBOD, and DO in each segment must be specified Values for DO should be 1 0 Only the particulate fraction of CBOD and NBOD will be subject to settling (Group J, Record 2, DISSF)

Transformation Parameters

This group of parameters includes spatially variable parameters, constants, and kinetic time functions for the water quality constituents being simulated Parameter values are entered for each segment Specified values for constants apply over the entire network for the whole simulation Kinetic time functions are composed of a series of values versus time in days

Water Temperature, °C-- Time and segment variable water temperatures can be specified using the parameters TMPSG and TMPFN and the time functions TEMP(1-4) If temperatures are to remain constant in time then the user should enter segment temperatures using the parameter TMPSG TMPFN and TEMP(1-4) should be omitted

If the user wants to enter time-variable temperatures, then values for the parameter TMPSG should be set to 1 0 The parameter TMPFN indicates which temperature function will be used by the model for each segment Values of 1 0 2 0 3 0, or 4 0 will call time functions TEMP(1), TEMP(2) TEMP(3) and TEMP(4), respectively Water temperatures should then be entered via these time functions as a series of temperature versus time values The product of TMPSG and the selected TEMP function will give the segment and time specific water temperatures used by EUTRO5

TMPSG and TMPFN are identified in EUTRO5 as parameters 3 and 4, respectively TEMP(1-4) are identified in EUTRO5 as time functions 1-4 (Group G, Record 4, PARAM(I,3), PARAM(I,4), Group I, Record 2, VALT(1-4,K))

Sediment Oxygen Demand, g/m^2-day-- Segment variable sediment oxygen demand fluxes and temperature coefficients can be specified using the parameters SOD1D and SODTA, respectively Values should be entered for water column segments that are in contact with the bottom of the water body If temperatures remain constant in time, then SODTA can be omitted (Group G, Record 4, PARAM(I 9) PARAM(I,11))

CBOD Deoxygenation Rate, day^{-1}-- The CBOD deoxygenation rate constant and temperature coefficient can be specified using constants KDC and KDT, respectively (Group H, Record 4, CONST(72), CONST(73))

NBOD Deoxygenation Rate, day^{-1}-- The NBOD deoxygenation rate constant and temperature coefficient can be specified using constants K12C and K12T respectively (Group H Record 4, CONST(11), CONST(12))

Reaeration Rate, day^{-1}-- There are three basic options for specifying reaeration -- a single rate constant segment and time variable rate constants, and flow and wind calculated rate constants These options are described in the Streeter-Phelps section

Full Linear DO Balance

The full DO balance equations divide the NBOD process into mineralization and nitrification and add the effects of photosynthesis and respiration from given phytoplankton levels

$$S_{k7} = -k_{71}\,\theta_{71}^{T-20}\,C_7 - \frac{v_{s3}}{D}(1 - f_{D7})\,C_7 \qquad 4\ 20$$

$$S_{k1} = +k_{71}\,\theta_{71}^{T-20}\,C_7 - k_{12}\,\theta_{12}^{T-20}\,C_1 \qquad 4\ 21$$

$$S_{k2} = +k_{12}\,\theta_{12}^{T-20}\,C_1 \qquad 4\ 22$$

$$S_{k5} = -k_d \, \theta_d^{T-20} \, C_5 - \frac{v_{S3}}{D} (1 - f_{D5}) \, C_5 \qquad 4\ 23$$

$$S_{k6} = +k_2 \, \theta_2^{T-20} \, (C_S - C_6) - k_d \, \theta_d^{T-20} \, C_5 - \frac{64}{14} k_{12} \, \theta_{12}^{T-20} \, C_1$$
$$- \frac{SOD}{D} \theta_S^{T-20} + (k_{1C}\theta_{1C}^{T-20} - k_{1R}\theta_{1R}^{T-20}) \frac{32}{12} C_4 \qquad 4\ 24$$

where S_{ki} is the source/sink term for variable i" in a segment, in mg/L-day   Kinetic rate constants and coefficients are as defined in Table 4 1   In addition, the following are used

k_{71} = organic nitrogen mineralization rate constant, day^{1}

θ_{71} = temperature coefficient

k_{1C} = average phytoplankton growth rate constant, day^{1} (user must input light and nutrient limited value)

θ_{1C} = temperature coefficient

f_{D7} = organic nitrogen dissolved fraction

Constant phytoplankton concentrations to be used in the DO balance are input under initial conditions as µg/L chlorophyll a If the carbon to chlorophyll ratio is not input then a default value of 30 is used   The particulate fractions of CBOD and ON are associated with transport field 3, organic matter settling

Environment Parameters

These parameters define the basic model identity including the segmentation, and control the simulation

Systems-- Select simulate' for NH3, NO3 CBOD DO, and ON Select constant for PHYT, and "bypass for PO4 and OP   (Group A, Record 4 NOSYS Record 9, SYSBY)

Segments-- Water column segments should be defined in the standard fashion   If CBOD or ON settling is to be simulated the user should add a single benthic segment underlying all water column segments   This benthic segment will merely act as a convenient sink for settling organic matter Model calculations within this benthic segment should be ignored (Group A Record 4, NOSEG Group C, Record 3, ISEG, IBOTSG, ITYPE, BVOL, DMULT)

Transport Parameters

This group of parameters define the advective and dispersive transport of model variables

Number of Flow Fields-- To simulate settling, the user should select solids 1 flow under advection The user should also select water column flow (Group D, Record 1, NFIELD)

Particulate Transport, m^3/sec-- Time variable settling and resuspension rates for particulate CBOD and ON can be input using the Solids 1 continuity array BQ and the time function QT For each solids flow field cross-sectional exchange areas (m^2) for adjacent segment pairs are input using the spatially-variable BQ Time-variable settling velocities can be specified as a series of velocities in m/sec versus time If the units conversion factor is set to 1 157e-5 then these velocities are input in units of m/day These velocities are multiplied internally by cross-sectional areas and treated as flows that carry particulate organic matter out of the water column (Group D, Record 4 BQ JQ, IQ, Record 6, QT, TQ)

Boundary Parameters

This group of parameters includes boundary concentrations waste loads, and initial conditions Boundary concentrations must be specified for any segment receiving flow inputs, outputs or exchanges Initial conditions include not only initial concentrations but also the density and solids transport field for each solid and the dissolved fraction in each segment

Boundary Concentrations, mg/L-- At each segment boundary, time variable concentrations must be specified for NH3 NO3, ON CBOD and DO A boundary segment is characterized by water exchanges from outside the network, including tributary inflows downstream outflows and open water dispersive exchanges (Group E Record 4, BCT)

Waste Loads, kg/day-- For each point source discharge time variable NH3, NO3, ON CBOD, and DO loads can be specified These loads can represent municipal and industrial wastewater discharges, or urban and agricultural runoff (Group F 1 Record 4, WKT)

Solids Transport Field-- The transport field associated with particulate CBOD and ON settling must be specified under initial conditions Field 3 is recommended for both (Group J, Record 1, IFIELD)

Solid Density, g/cm -- A value of 0 can be entered for the nominal density of NH3, NO3, ON, CBOD, and DO This information is not used in EUTRO5 (Group J, Record 1, DSED)

Initial Concentrations, mg/L-- Concentrations of NH3, NO3, ON, CBOD, and DO in each segment must be specified for the time at which the simulation begins Average concentrations of PHYT expressed as μg/L chlorophyll a, must be specified as well These are converted to mg/L phytoplankton carbon in EUTRO5 using a default carbon to chlorophyll ration of 30 Phytoplankton concentrations will remain constant throughout the simulation and affect DO through photosynthesis and respiration Concentrations of zero for non-simulated variables -- PO4 and OP -- will be entered by the preprocessor (Group J, Record 2, C)

Dissolved Fraction-- The dissolved fraction of NH3, NO3, ON, CBOD and DO in each segment must be specified Values for DO should be 1 0 Only the particulate fraction of CBOD and ON will be subject to settling (Group J, Record 2, DISSF)

Transformation Parameters

This group of parameters includes spatially variable parameters, constants, and kinetic time functions for the water quality constituents being simulated Parameter values are entered for each segment Specified values for constants apply over the entire network for the whole simulation Kinetic time functions are composed of a series of values versus time in days

Water Temperature, °C-- Time and segment variable water temperatures can be specified using the parameters TMPSG and TMPFN, and the time functions TEMP(1-4), as described in the modified Streeter-Phelps section

Sediment Oxygen Demand, g/m^2-day-- Segment variable sediment oxygen demand fluxes and temperature coefficients can be specified using the parameters SOD1D and SODTA respectively Values should be entered for water column segments that are in contact with the bottom of the water body (Group G Record 4 PARAM(I 9), PARAM(I 12))

Nitrogen Mineralization Rate, day^{-1}-- The mineralization rate constant and temperature coefficient for dissolved organic nitrogen can be specified using constants K71C and K71T respectively (Group H Record 4, CONST(91), CONST(92))

Nitrification Rate, day^{-1}-- The nitrification rate constant and temperature coefficient for dissolved ammonia nitrogen can be specified using constants K12C and K12T, respectively (Group H Record 4, CONST(11), CONST(12))

CBOD Deoxygenation Rate, day^{-1} -- The CBOD deoxygenation rate constant and temperature coefficient can be specified using constants KDC and KDT, respectively (Group H, Record 4, CONST(72), CONST(73))

Reaeration Rate, day^{-1}-- There are three basic options for specifying reaeration -- a single rate constant, segment and time variable rate constants, and flow and wind calculated rate constants These options are described in the Streeter-Phelps section

Photosynthesis Rate, day^{-1}-- The average phytoplankton growth rate constant and temperature coefficient can be input using constants K1C and K1T, respectively For DO balance simulations where phytoplankton dynamics are bypassed the growth rate constant must reflect average light and nutrient limitations in the water body (Group H, Record 4, CONST(41), CONST(42))

Respiration Rate, day^{-1}-- The average phytoplankton respiration rate constant and temperature coefficient can be input using constants K1RC and K1RT respectively (Group H, Record 4, CONST(50), CONST(51))

Nonlinear DO Balance

The nonlinear DO balance equations add feedback from DO concentratons to terms in the linear DO balance equations presented above This feedback can become important in inhibiting nitrification and carbonaceous oxidation and in promoting denitrification where low DO concentrations occur

For this level of analysis, the linear DO balance equations presented above are supplemented with nonlinear terms for carbonaceous oxidation, nitrification, and denitrification These terms are presented in Figure 4 2 and Table 4 1 The environment transport and boundary parameters required to implement the nonlinear DO balance are the same as those in the linear DO balance presented above The user should supplement the transformation parameters presented above with the following

Nitrification Rate, day^{-1}-- The nitrification rate constant and temperature coefficient for dissolved ammonia nitrogen can be specified using constants K12C and K12T respectively The half-saturation constant for oxygen limitation of nitrification can be specified using constant KNIT The default value for KNIT is

0 0, indicating no oxygen limitation (Group H, Record 4 CONST(11), CONST(12) CONST(13))

Denitrification Rate, day^{-1}-- The denitrification rate constant and temperature coefficient for dissolved nitrate nitrogen can be specified using constants K20C and K20T, respectively The half-saturation constant for oxygen limitation of denitrification can be specified using constant KNO3 The default value for KNO3 is 0 0, indicating no denitrification at oxygen concentrations above 0 0 (Group H, Record 4, CONST(21) CONST(22), CONST(23))

CBOD Deoxygenation Rate, day^{-1}-- The CBOD deoxygenation rate constant and temperature coefficient can be specified using constants KDC and KDT, respectively The half-saturation constant for oxygen limitation of carbonaceous deoxygenation can be specified using constant KBOD The default value for KBOD is 0 0 indicating no oxygen limitation (Group H, Record 4 CONST(72), CONST(73), CONST(75))

Data Group Descriptions

Input datasets to simulate DO balance in a river are given with the model software A comprehensive listing of the WASP5 data groups, records and variables is given in Part B of this documentation

CHAPTER 5

EUTROPHICATION

5 1 MODEL DESCRIPTION

Introduction

Nutrient enrichment and eutrophication are continuing concerns in many water bodies High concentrations of nitrogen and phosphorus can lead to periodic phytoplankton blooms and an alteration of the natural trophic balance Dissolved oxygen levels can fluctuate widely, and low DO concentrations in bottom waters can result

Eutrophication has been modeled for approximately 30 years The equations implemented here were derived from the Potomac Eutrophication Model, PEM (Thomann and Fitzpatrick 1982) and are fairly standard Sections of this text are modified from the PEM documentation report

Overview of WASP5 Eutrophication

The nutrient enrichment eutrophication, and DO depletion processes are simulated using the EUTRO5 program Several physical-chemical processes can affect the transport and interaction among the nutrients, phytoplankton, carbonaceous material and dissolved oxygen in the aquatic environment Figure 5 1 presents the principal kinetic interactions for the nutrient cycles and dissolved oxygen

EUTRO5 can be operated by the user at various levels of complexity to simulate some or all of these variables and interactions Four levels for simulating the DO balance were described in Chapter 4 Three levels of complexity for simulating eutrophication are identified and documented at the end of this section (1) simple eutrophication kinetics (2) intermediate eutrophication kinetics, and (3) intermediate eutrophication kinetics with benthos The user should become familiar with the full capabilities of EUTRO5 even if simpler simulations are planned

EUTRO5 simulates the transport and transformation reactions of up to eight state variables, illustrated in Figure 5 1 They can be considered as four interacting systems phytoplankton kinetics, the phosphorus cycle, the nitrogen cycle, and the dissolved oxygen balance The general WASP5 mass balance

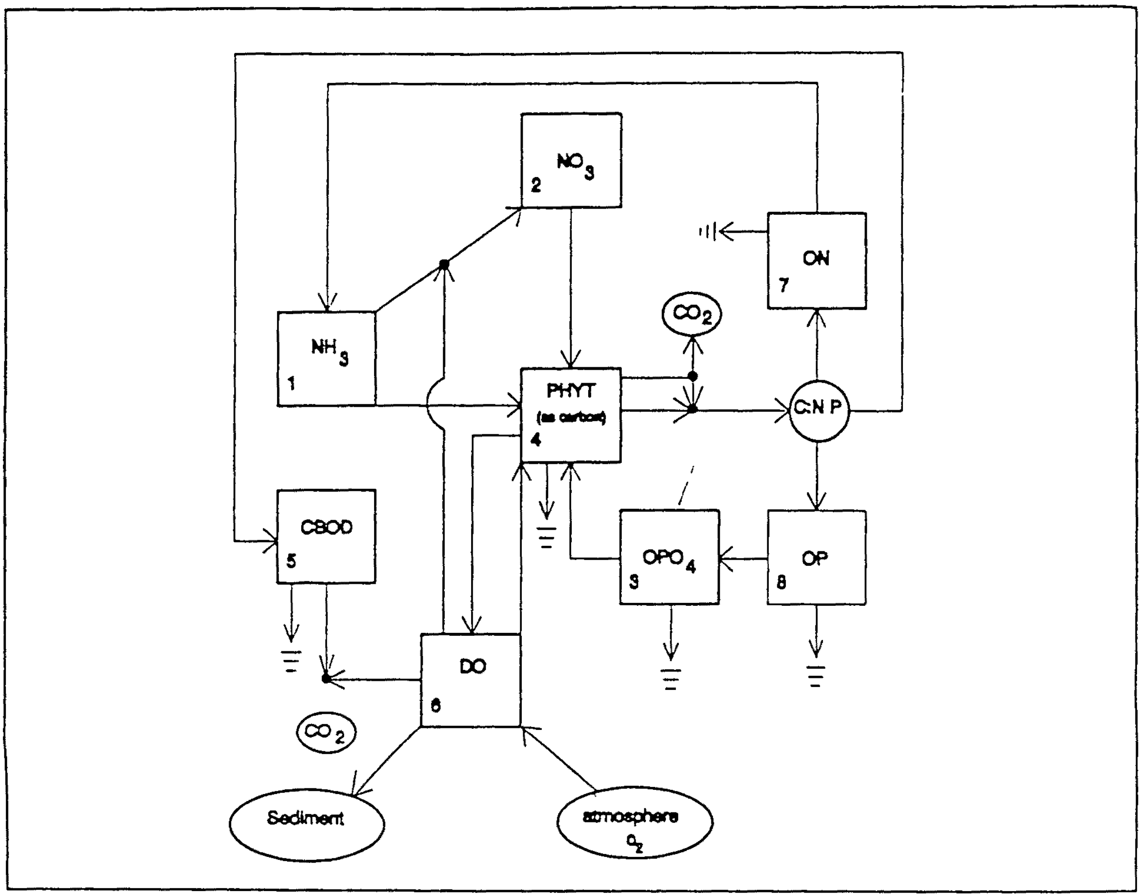


Figure 5 1 EUTRO5 state variable interactions

equation is solved for each state variable To this general equation the EUTRO5 subroutines add specific transformation processes to customize the general mass balance for the eight state variables in the water column and benthos Following a short summary of the material cycles the rest of Section 5 1 covers the specific details for the several transformation sources and sinks

Phosphorus Cycle

Dissolved or available inorganic phosphorus (DIP) interacts with particulate inorganic phosphorus via a sorption-desorption mechanism DIP is taken up by phytoplankton for growth, and is incorporated into phytoplankton biomass Phosphorus is returned from the phytoplankton biomass pool to dissolved and particulate organic phosphorus and to dissolved inorganic phosphorus through endogenous respiration and nonpredatory mortality Organic phosphorus is converted to dissolved inorganic phosphorus at a temperature-dependent mineralization rate

Nitrogen Cycle

The kinetics of the nitrogen species are fundamentally the same as the phosphorus system Ammonia and nitrate are taken up by phytoplankton for growth and incorporated into phytoplankton biomass The rate at which each is taken up is a function of its concentration relative to the total inorganic nitrogen (ammonia plus nitrate) available Nitrogen is returned from the phytoplankton biomass pool to dissolved and particulate organic nitrogen and to ammonia through endogenous respiration and nonpredatory mortality Organic nitrogen is converted to ammonia at a temperature dependent mineralization rate, and ammonia is then converted to nitrate at a temperature- and oxygen-dependent nitrification rate Nitrate may be converted to nitrogen gas in the absence of oxygen at a temperature- and oxygen-dependent denitrification rate

Dissolved Oxygen

Dissolved oxygen is coupled to the other state variables The sources of oxygen considered are reaeration and evolution by phytoplankton during growth The sinks of oxygen are algal respiration, oxidation of detrital carbon and carbonaceous material from waste effluents and nonpoint discharges, and nitrification These processes are discussed in Chapter 4

Phytoplankton Kinetics

Phytoplankton kinetics assume a central role in eutrophication affecting all other systems An overview of this system is given in Figure 5 2

It is convenient to express the reaction term of phytoplankton S_{k4j}, as a difference between the growth rate of phytoplankton and their death and settling rates in the volume V_j That is

$$S_{k4j} = (G_{p1j} - D_{p1j} - k_{s4j}) \ P_j \qquad 5\ 1$$

where

S_j = reaction term, mg carbon/L-day

P_j = phytoplankton population, mg carbon/L

G_{p1j} = growth rate constant, day^{1}

D_j = death plus respiration rate constant, day^{1}

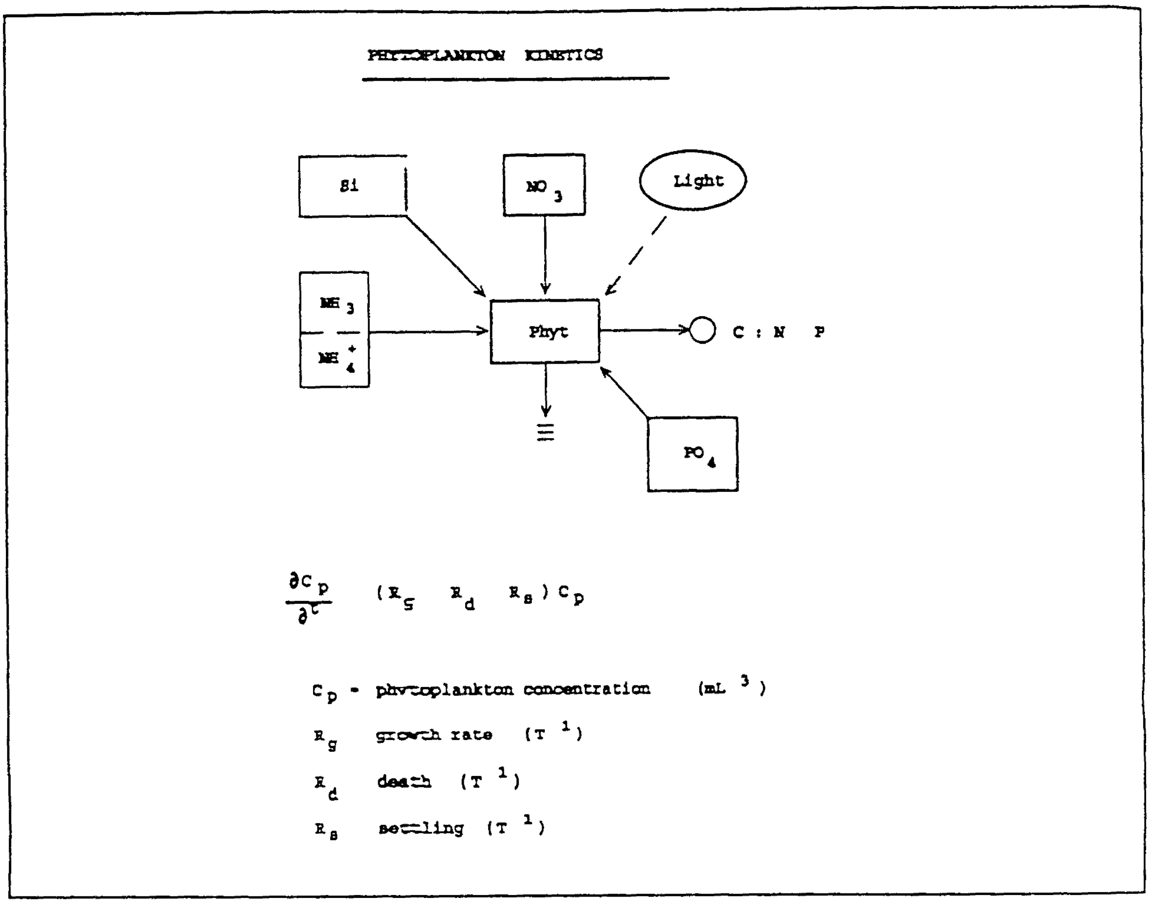


Figure 5 2 Phytoplankton kinetics

k_{s4j} = settling rate constant, day^1

j = segment number unitless

The subscript 1 identifies the quantities as referring to phytoplankton type 1, (only one type is considered in this particular model) the subscript j refers to the volume element being considered The balance between the magnitude of the growth rate and death rate (together with the transport settling and mixing) determines the rate at which phytoplankton mass is created in the volume element V_j In subsequent text and in figures subscripts 1 and j will be omitted unless needed for clarity

Phytoplankton Growth

The growth rate of a population of phytoplankton in a natural environment is a complicated function of the species of phytoplankton present and their differing reactions to solar radiation temperature, and the balance between nutrient availability and phytoplankton requirements The available information is not sufficiently detailed to specify the growth kinetics for individual algal species in a natural environment Rather than considering the problem of different species and their associated environmental and nutrient requirements, this model characterizes the population as a whole by the total biomass of the phytoplankton present

A simple measure of total biomass that is characteristic of all phytoplankton, chlorophyll *a*, is used as the aggregated variable The principal advantages are that the measurement is direct, it integrates cell types and ages and it accounts for cell viability The principal disadvantage is that it is a community measurement with no differentiation of functional groups (e g diatoms, blue-greens) also, it is not necessarily a good measurement of standing crop in dry weight or carbon units because the chlorophyll-to-dry-weight and carbon ratios are variable and non-active chlorophyll (phaeopigments) must be measured to determine viable chlorophyll concentrations

As can be seen from the above discussion, no simple aggregate measurement is entirely satisfactory From a practical point of view, the availability of extensive chlorophyll data essentially dictates its use as the aggregate measure of the phytoplankton population or biomass for calibration and verification purposes For internal computational purposes however EUTRO5 uses phytoplankton carbon as a measure of algal biomass Using either a fixed or variable carbon to chlorophyll mechanism (discussed subsequently), phytoplankton chlorophyll *a* may be computed and used as the calibration and verification variable to be compared against observed chlorophyll *a* field data

With a choice of biomass units established a growth rate that expresses the rate of production of biomass as a function of the important environmental variables (temperature light, and nutrients) may be developed The specific growth rate G_{P1j} in segment j is related to k_{1c}, the maximum 20°C growth rate at optimum light and nutrients, via the following equation

$$G_{P1j} = k_{1c}\, X_{RTj}\, X_{RIj}\, X_{RNj} \qquad 5\ 2$$

where

X_{RTj} = the temperature adjustment factor dimensionless

X_{RIj} = the light limitation factor as a function of I f D, and K_e, dimensionless

X_{RJ} = the nutrient limitation factor as a function of dissolved inorganic phosphorus and nitrogen (DIP and DIN), dimensionless

T = ambient water temperature, °C

I = incident solar radiation, ly/day

f = fraction day that is daylight, unitless

D = depth of the water column or model segment, m

K_e = total light extinction coefficient, m^{-1}

DIP = dissolved inorganic phosphorus (orthophosphate) available for growth, mg/L

DIN = dissolved inorganic nitrogen (ammonia plus nitrate) available for growth, mg/L

An initial estimate of k_{1c} can be made based upon previous studies of phytoplankton dynamics and upon reported literature values (such as Bowie et al 1985) and subsequently refined during the calibration and verification process This maximum growth rate constant is adjusted throughout the simulation for ambient temperature, light, and nutrient conditions

Temperature -- Water temperature has a direct effect on the phytoplankton growth rate The selected maximum growth rate is temperature-corrected using temporally- and spatially-variable water column temperatures as reported in field studies The temperature correction factor is computed using

$$X_{RTJ} = \theta_{1c}^{T-20} \qquad 1.08 \tag{5 3}$$

where

θ_{1c} = temperature coefficient, unitless

Light -- In the natural environment, the light intensity to which the phytoplankton are exposed is not uniformly at the optimum value At the surface and near-surface of the air-water interface photoinhibition can occur at high light intensities, whereas at depths below the euphotic zone light is not available for photosynthesis due to natural and algal-related turbidity

Modeling frameworks developed by Di Toro (1971), and by Smith (1980) extending upon a light curve analysis formulated by Steele (1962) account for both the effects of supersaturating light intensities and light attenuation through the water column The instantaneous depth-averaged growth rate reduction developed by Di Toro is presented in Equation 5 4 and is obtained by integrating the specific growth rate over depth

$$\overline{X_{RI}} = \frac{e}{K_e\ D} f\ \left[\exp\left\{-\frac{I_a}{I_s}\exp(-K_e\ D)\right\} - \exp\left(-\frac{I_a}{I_s}\right)\right] \qquad 5\ 4$$

where

I_a = the average incident light intensity during daylight hours just below the surface assumed to average 0 9 I/f, ly/day

I_s = the saturating light intensity of phytoplankton, ly/day

K_e = the light extinction coefficient, computed from the sum of the non-algal light attenuation, K_e' and the phytoplankton self-shading attenuation, K_{eshd} (as calculated by Equation 5 5), m^{-1}

$$K_{eshd} = 0\ 0088\, P_{Chl} + 0\ 054\, P_{Chl}^{0\ 67} \qquad 5\ 5$$

and P_{Chl} = phytoplankton chlorophyll concentration µg/L

Typical clear sky values of surface light intensity for different latitudes and months are provided in Table 5 1

Equation 5 4 is quite similar in form to that developed by Smith, which is also available as an option in this model

$$\overline{X_{RI}}(t) = \frac{e}{K_e\ D}\left[\exp\left\{-\frac{I_o}{I_s}\exp(-K_e\ D)\right\} - \exp\left(-\frac{I_o}{I_s}\right)\right] \qquad 5\ 6$$

where

$$\begin{aligned} I_o(t) &= \left(\frac{\pi}{2}\frac{I}{f}\right) SIN\left(\frac{\pi\ t}{f}\right), & t &= 0 - f \\ &= 0, & t &= f - 1 \end{aligned} \qquad 5\ 7$$

Table 5 1 Calculated Solar Radiant Energy Flux to a Horizontal Surface Under a Clear Sky (langleys/day)

[illegible] 24 6°

Latitude	Time of Day	Season				Annual Mean
		Spring	Summer	Fall	Winter	
30祇	Mean[1]	680	750	530	440	600
	Mid-Day[2]	2100	2200	1700	1400	1900
40祇	Mean	650	740	440	320	540
	Mid-Day	1900	2100	1400	1000	1600
50祇	Mean	590	710	330	190	460
	Mid-Day	1700	1900	1000	650	1300

[1] calculated seasonal means under a clear sky, representing upper limits for solar radiant energy at sea level Reference Weast and Astle (1980)

[2] Mid-day flux extended over a 24-hour period, assuming an atmospheric turbidity of 0 precipitable water content of 2 cm, and an atmospheric ozone content of 34 cm NTP Reference Robinson (1966)

and

$$I_B = \frac{k_{1c}\, X_{RT}\, \theta_c\, e}{\Phi_{max}\, K_c\, f_u} \qquad 5\ 8$$

where

I_o = the time variable incident light intensity just below the surface, assumed to follow a half sin function over daylight hours, ly/day

Φ_{max} = the quantum yield, mg carbon fixed per mole of light quanta absorbed

K_c = the extinction coefficient per unit of chlorophyll, m²/mg chlorophyll *a*

K_e = the light extinction coefficient, computed from the sum of the non-algal light attenuation K_o , and the phytoplankton self-shading attenuation, K_{eshd} (as calculated by Equation 5 9), m ^{1}

$$K_{eshd} = K_c \, P_{Chl} \qquad 5\ 9$$

f_u = units conversion factor (0 083, assuming 43% incident light is visible and 1 mole photons is equivalent to 52,000 cal), mole photons/m^2-ly

θ_c = the ratio of carbon to chlorophyll in the phytoplankton, (mg carbon/mg chlorophyll *a*)

e = the base of natural logarithms (2 71828), unitless

Equations 5 6 - 5 9 give a light limitation coefficient that varies over the day with incident light This term is numerically integrated over the day within the computer program to obtain daily average light limitation

$$\overline{X_{RI}} = \int_0^1 X_{RI}(t)\, dt \qquad 5\ 10$$

The term I_s, the temperature-dependent light saturation parameter is an unknown in the Di Toro light formulation and must be determined via the calibration-verification process In the Smith formulation, this term is calculated from parameters that are reasonably well documented in the literature As Smith (1980) points out, since the early experiments of Warburg and Negelein (1923), maximum photosynthetic quantum yield (Φ_{max}) has been measured for a wide range of conditions (reviewed by Kok, 1960) and a nearly temperature-independent value of 0 08 to 0 1 mole O_2 per mole of photons absorbed is now widely accepted for photosynthesizing plants in general in the laboratory Bannister (1974a) gives good arguments for adopting 0 06 mole carbon (0 07 mole O_2) per mole of photons as the maximum yield for plankton in nature Reported values for K_c generally fall in the range 0 01 to 0 02 r mg ^{1} and 0 016 m^{2}mg ^{1} has been suggested as the approximate average (Bannister, 1974b)

A second feature incorporated in the modeling framework derived from Smith s work is the calculation of a variable carbon to chlorophyll ratio based on the assumption that adaptive changes in carbon to chlorophyll occur so as to maximize the specific growth rate for ambient conditions of light and temperature Smith found that phytoplankton adjust chlorophyll composition so that I_s roughly equals 30% of the average available light The expression used to calculate the carbon to chlorophyll ratio is presented in Equation 5 11

$$\theta_c = 0\ 3 \quad \frac{\Phi_{max}\, K_c\, f_u}{k_{1c}\, X_{RT}\, e} \quad I_a \left[\frac{1 - e^{-K_e D}}{K_e\, D}\right] \qquad 5\ 11$$

where the latter term is the average daily solar radiation within a segment during daylight hours, in ly/day Note that substituting Equation 5 11 into 5 8 gives an I_s equal to 30% of the average available light

A review of reported carbon/chlorophyll ratios in nature (Eppley and Sloane, 1966) suggests that physiological factors (in part the energy cost of synthesizing chlorophyll as compared with other cellular compounds) come into play to prevent θ_c from going much below 20 even in very low light This lower limit of 20 has been included when determining a value for θ_c Previously reported values of θ_c from algal composition studies conducted by EPA Region III's Central Regional Laboratory (CRL) are compared in Table 5 2 to calculated values of using Equation 5 11 There is general agreement between the measured and calculated values Unfortunately, no winter algae composition studies were available for comparison purposes

Nutrients -- The effects of various nutrient concentrations on the growth of phytoplankton have been investigated and the results are quite complex As a first approximation to the effect of nutrient concentration on the growth rate it is assumed that the phytoplankton population in question follows Monod growth kinetics with respect to the important nutrients That is, at an adequate level of substrate concentration the growth rate proceeds at the saturated rate for the ambient temperature and light conditions present At low substrate concentration, however, the growth rate becomes linearly proportional to substrate concentration Thus for a nutrient with concentration N in the j^{th} segment, the factor by which the saturated growth rate is reduced is $\boxed{N_j/(K_j + N_j)}$. The constant K_j (called the Michaelis or half-saturation constant) is the nutrient concentration at which the growth rate is half the saturated growth rate Because there are two nutrients, nitrogen and phosphorus considered in this framework, the Michaelis-Menten expression is evaluated for the dissolved inorganic forms of both nutrients and the minimum value is chosen to reduce the saturated growth rate, as given by Equation 5 12

Table 5 2 Carbon to Chlorophyll a Ratio

Sampling Period	Carbon/Chlorophyll a μg 痢 C/痢 Chlorophyll a Observed Mean	 Observed Range	 Predicted Range
July 20-Oct 6 1970[1]	45	25-68	24-28
August 1-29, 1977[2]	28	12-37	23-26
Sept 7-28, 1978[2]	21	15-27	26-30
Sept 7-28 1978[3]		26-30	

1 Elemental analysis of blue-green algae
2 Laboratory elemental analysis of overall phytoplankton population
3 Estimates of cell composition based upon field data

$$X_{RN} = Min\left(\frac{DIN}{K_{mN} + DIN}, \frac{DIP}{K_{mP} + DIP}\right) \qquad 5\ 12$$

At the user's discretion, the multiplicative formulation for nutrient limitation may be selected This formulation multiplies the two terms in 5 12 It is not generally recommended

Figure 5 3 presents plots of G(N) versus DIN and DIP with K_{mN} = 25 痢-N/L and K_{mP} = 1 痢-P/L, respectively The upper plot shows the standard Michaelis-Menten response curve to various concentrations of the inorganic nutrients As can be seen, no significant reduction in growth rate is achieved until DIN is less than 200 痢/L (0 2 mg/l) or until DIP is less than 8 痢/L (0 008 mg/l)

The lower plot on Figure 5 3 uses an expanded nutrient scale and shows the Michaelis-Menten formulation in a slightly different format Here the impact of the function may be evaluated quite readily For example, a particular reach of the water body may have concentrations of DIN equal to 100 痢/L This corresponds to a 20% reduction in the growth rate (X_{RN} = 0 8) In order for phosphorus to become the limiting nutrient in the same reach, dissolved inorganic phosphorus must reach a level

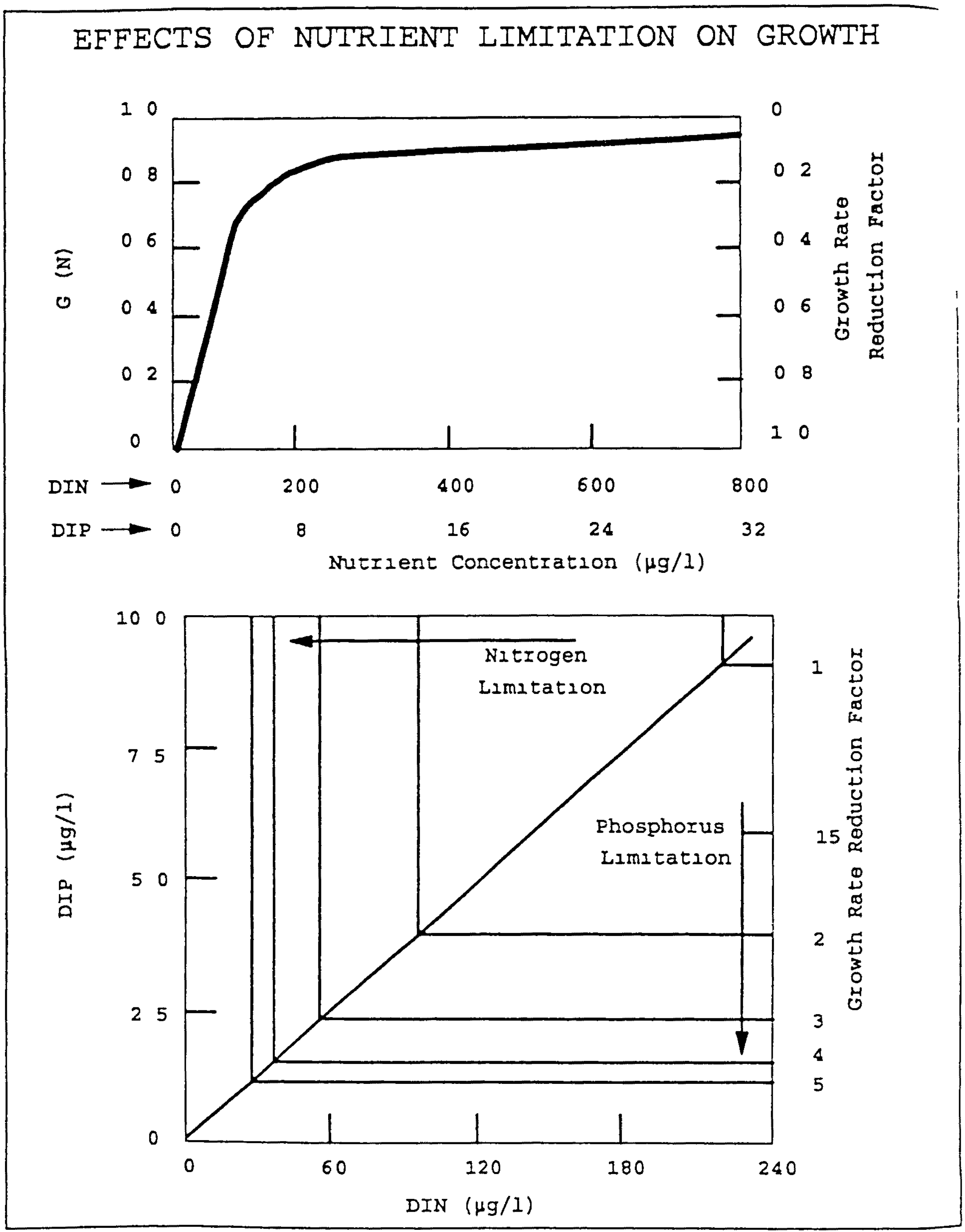


Figure 5 3 Effects of nutrient limitation on growth rate assuming K_{mn} = 25 痢-N/L $K_{-,}$ = 1 痢-P/L of 4 痢/L or less It should also be noted that if upstream nitrogen controls were instituted such that DIN was reduced to 60 痢/L for that same reach then a further reduction in DIP to 2 5 痢/L would be required to keep phosphorus as the limiting nutrient In other words as water column concentrations of DIP begin to approach growth limiting levels due to continued reduction in point source phosphorus effluents, any nitrogen control strategies that might be instituted would require additional levels of phosphorus removal in order to keep phosphorus as the limiting nutrient

Phytoplankton Death

Numerous mechanisms have been proposed that contribute to the biomass reduction rate of phytoplankton endogenous respiration, grazing by herbivorous zooplankton, and parasitization The first two mechanisms have been included in previous models for phytoplankton dynamics, and they have been shown to be of general importance

The endogenous respiration rate of phytoplankton is the rate at which the phytoplankton oxidize their organic carbon to carbon dioxide per unit weight of phytoplankton organic carbon Respiration is the reverse of the photosynthesis process and, as such, contributes to the reduction in the biomass of the phytoplankton population If the respiration rate of the phytoplankton as a whole is greater than the growth rate, there is a net loss of phytoplankton carbon or biomass The endogenous respiration rate is temperature dependent (Riley, 1949) and is determined via Equation 5 13

$$k_{1R}(T) = k_{1R}(20^\circ C)\ \theta_{1R}^{(T-20)} \qquad 5\ 13$$

where

k_{1R}(20蚓) = the endogenous respiration rate at 20蚓 °C day^{1}

$k_{1D}(T)$ = the temperature corrected rate day^{1}

θ_{1D} = temperature coefficient, dimensionless

Reported values of endogenous respiration at 20 C vary from 0 02 day^{1} to 0 60 day^{1} with most values falling between 0 05 day^{1} and 0 20 day^{1} (Bowie et al , 1985) Di Toro and Matystik (1980) report a value of 1 045 for θ_{1P} The total biomass reduction rate for the phytoplankton in the jth segment is expressed via Equation 5 14

$$D_{1j} = k_{1R}(T) + k_{1D} + k_{1G} Z(t) \qquad 5\ 14$$

where

D_{1j} = biomass reduction rate, day^{-1}

k_{1D} = death rate, representing the effect of parasitization, i e , the infection of algal cells by other microorganisms, and toxic materials, such as chlorine residual, day^{-1}

k_{1G} = grazing rate on phytoplankton per unit zooplankton population, L/mgC-day

$Z(t)$ = herbivorous zooplankton population grazing on phytoplankton, mgC/L

Note that the zooplankton population dynamics are described by the user, not simulated If population fluctuations are important in controlling phytoplankton levels in a particular body of water, the user may want to simulate zooplankton and their grazing On the other hand, many studies need only a constant first order grazing rate constant, where grazing rates are assumed proportional to phytoplankton levels In that case, k_{1G} can be set to the first order constant with Z(t) omitted (default value = 1) Reported grazing rates vary from 0 1 to 1 5 L/mgC-day (Bowie et al , 1985)

Phytoplankton Settling

The settling of phytoplankton is an important contribution to the overall mortality of the phytoplankton population, particularly in lakes and coastal oceanic waters Published values of the settling velocity of phytoplankton, mostly under quiescent laboratory conditions, range from 0 07-18 m/day In some instances however the settling velocity is zero or negative Actual settling in natural waters is a complex phenomenon, affected by vertical turbulence, density gradients, and the physiological state of the different species of phytoplankton Although the effective settling rate of phytoplankton is greatly reduced in a relatively shallow well mixed river or estuary due to vertical turbulence it still can contribute to the overall mortality of the algal population In addition, the settling phytoplankton can be a significant source of nutrients to the sediments and can play an important role in the sediment oxygen demand. In EUTRO5, phytoplankton are equated to solid type 2 Time and segment-variable phytoplankton settling velocities can be input by the user then, using transport field 4, so that

Table 5 3 Phytoplankton Net Growth Terms

Description	Notation	Values	Units	
	Exogenous Variables			
Extinction Coefficient	K_e	0 1-5	m^{-1}	
Segment Depth	D	0 1-30	m	
Water Temperature	T	0-35	°C	
Fraction of day that is daylight	f	0 3-0 7	-	
Average Daily Surface Solar Radiation	I_a	200-750	langleys/day	
Zooplankton Population	Z	0	mgC/L	
	Rate Constants			
Maximum Growth Rate	k_{1c}	2 0 (1 3~2 5)	day^{-1}	K1C
Temperature Coefficient	θ_{1c}	1 068	none	K1T
Maximum Photosynthetic Quantum Yield	Φ_{max}	720 0	mg C/mole photon	PHI
Phytoplankton Self-Light Attenuation	K_c	0 01~0 02 0 017	m^2/mg Chl a	KC
Carbon-Chlorophyll Ratio	θ_c	20-50	-	CCHL
Saturating Light Intensity	I_s	200-500	langleys/day	IS1
Half-Saturation Constant for Nitrogen	K_{mN}	25 0	μg N/L	KMNG1
Half-Saturation Constant for Phosphorus	K_{mP}	1 0 0 5~2 0	μg P/L	KMPG1
Endogenous Respiration	k_{1R}	0 125 0 5~0 20	day^{-1}	K1RC
Temperature Coefficient	θ_{1R}	1 045	none	K1RT
Settling Velocity	v_{s4}	0 1	m/day	
Death Rate	k_{1D}	0 02	day^{-1}	K1D
Grazing Rate	k_{1G}	0 0 1~1 5 (Bowie et al 1985)	L/mgC-day	K1G

$$k_{s4j} = \frac{v_{s4ij}}{D_j} \qquad 5\ 15$$

where

k_{s4j} = the effective phytoplankton settling or loss rate day^{1}

v_{s4ij} = the net settling velocity of phytoplankton from segment j to segment i, m/day

D_j = depth of segment j, equal to volume/surface area m

Summary

This completes the specification of the growth and death rates of the phytoplankton population in terms of the physical variables light, temperature, and the nutrient concentrations present Table 5 3 summarizes the variables and parameters in the net growth equations With these variables known as a function of time, it is possible to calculate the phytoplankton chlorophyll throughout the year

The nutrients are not known a priori however, because they depend upon the phytoplankton population that develops These systems are interdependent and cannot be analyzed separately It is necessary to formulate a mass balance for the nutrients as well as the phytoplankton in order to calculate the chlorophyll that would develop for a given set of environmental conditions

Stoichiometry and Uptake Kinetics

A principal component in the mass-balance equations written for the nutrient systems included in the eutrophication framework is the nutrient uptake kinetics associated with phytoplankton growth To specify the nutrient uptake kinetics associated with this growth however it is necessary to specify the population stoichiometry in units of nutrient uptake/mass of population synthesized For carbon as the unit of population biomass the relevant ratios are the mass of nitrogen and phosphorus per unit mass of carbon A selection of these ratios presented by Di Toro et al (1971) indicates that their variability is quite large The use of constant ratios in the analysis, then, is questionable

Upon further investigation, however, it is clear that the reason these ratios vary is the varying cellular content of nutrients, which is, in turn, a function of the external nutrient concentrations and the past history of the phytoplankton population Large ratios of carbon to nitrogen or phosphorus correspond to that nutrient limiting growth, small ratios reflect excess nutrients Thus, the choice of the relevant ratios can be made with the specific situation in mind

The operational consequence of this choice is that the population stoichiometry under non-limiting conditions may be underestimated, but under limiting conditions should be estimated correctly Hence the trade off is a probable lack of realism during a portion of the year versus a correct estimate of phytoplankton biomass during periods of possible nutrient limitations Because this is usually the critical period and because most questions to be answered are usually sensitive to maximum summer populations, this choice is a practical expedient A comparison of carbon-to-nitrogen and carbon-to-phosphorus ratios measured in the Potomac Estuary is provided in Table 5 4

Table 5 4 Phosphorus-to-Carbon and Nitrogen-to-Carbon Ratios

	Phosphorus/Carbon mg P/mg C		Nitrogen/Carbon mg N/mg C	
Sampling Period	Observed Mean	Observed Range	Observed Mean	Observed Range
July 20-Oct 6 1970[1]	0 023	0 010-0 046	0 26	0 10-0 48
August 1-29, 1977[3]	0 024	0 012-0 028	0 24	0 15-0 36
Sept 7-28, 1978[2]	0 030	0 017-0 047	0 26	0 18-0 35
Sept 7-28 1978[2]	0 031		0 26	
Model	0 025		0 25	

1 Elemental analysis of blue-green algae
2 Laboratory elemental analysis of overall phytoplankton population
3 Estimates of cell composition based upon field data

Once the stoichiometric ratios have been determined, the mass balance equations may be written for the nutrients in much the same way as is done for the phytoplankton biomass The primary interaction between the nutrient systems and the phytoplankton system is the reduction or sink of nutrients associated with phytoplankton growth A secondary interaction occurs wherein the phytoplankton system acts as a source of nutrients due to release of stored cellular nitrogen and phosphorus during algal respiration and death

The Phosporus Cycle

Three phosphorus variables are modeled phytoplankton phosphorus, organic phosphorus, and inorganic (orthophosphate) phosphorus Organic phosphorus is divided into particulate and dissolved concentrations by spatially variable dissolved fractions Inorganic phosphorus also is divided into particulate and dissolved concentrations by spatially variable dissolved fractions, reflecting sorption The phosphorus equations are summarized in Figure 5 4

1. *PHYTOPLANKTON PHOSPHORUS*

$$\frac{\partial (C_4 a_{pc})}{\partial t} = \underbrace{G_{P1} a_{pc} C_4}_{growth} - \underbrace{D_{P1} a_{pc} C_4}_{death} - \underbrace{\frac{v_{s4}}{D} a_{pc} C_4}_{settling}$$

2. *ORGANIC PHOSPHORUS*

$$\frac{\partial C_8}{\partial t} = \underbrace{D_{P1} a_{pc} f_{op} C_4}_{death} - \underbrace{k_{83} \theta_{83}^{T-20} \left(\frac{C_4}{K_{mPc} + C_4} \right) C_8}_{mineralization} - \underbrace{\frac{v_{s3} (1 - f_{D8})}{D} C_8}_{settling}$$

3. *INORGANIC PHOSPHORUS*

$$\frac{\partial C_3}{\partial t} = \underbrace{D_{P1} a_{pc} (1 - f_{op}) C_4}_{death} + \underbrace{k_{83} \theta_{83}^{T-20} \left(\frac{C_4}{K_{mPc} + C_4} \right) C_8}_{mineralization} - \underbrace{G_{P1} a_{pc} C_4}_{growth}$$

Figure 5 4 Phosphorus cycle equations

Table 5 5 presents the reaction rate terms used in the Potomac study

Phytoplankton Growth

As phytoplankton grow dissolved inorganic phosphorus is taken up, stored and incorporated into biomass For every mg of phytoplankton carbon produced, a_{PC} mg of inorganic phosphorus is taken up

Phytoplankton Death

As phytoplankton respire and die, biomass is recycled to

Table 5 5 Phosphorus Reaction Terms (Potomac Study)

Description	Notation	Value	Units
Phytoplankton biomass as carbon	P_c	-	mg C/L
Specific phytoplankton growth rate	G_{pij}	(eq 5 2)	day ^{1}
Phytoplankton loss rate	D_{pij}	(eq 5 14)	day ^{1}
Phosphorus to carbon ratio	a_{PC}	0 025	mg P/mg C PCRC
Dissolved organic phosphorus mineralization at 20°C	k_{83}	0 22	day ^{1} K83C
Temperature coefficient	θ_{83}	1 08	none K83T
Half saturation constant for phytoplankton limitation of phosphorus recycle	K_{mPc}	1 0	mg C/L KMPC
Fraction of dead and respired phytoplankton recycled to the organic phosphorus pool	f_{op}	0 5	none FOP
recycled to the phosphate phosphorus pool	$(1-f_{op})$	0 5	none
Fraction dissolved inorganic phosphorus in the water column	f_{D3}	0 85, 0 70	none
Fraction dissolved organic phosphorus	f_{D8}	-	none
Organic matter settling velocity	v_{s3}	-	m/day
Inorganic sediment settling velocity	v_{s5}	-	m/day

nonliving organic and inorganic matter For every mg of phytoplankton carbon consumed or lost, a_{PC} mg of phosphorus is released A fraction f_{op} is organic while $(1 - f_{op})$ is in the inorganic form and readily available for uptake by other viable algal cells In work on the Great Lakes, f_{op} was assigned at 50% (Di Toro and Matystik, 1980)

Mineralization

Nonliving organic phosphorus must undergo mineralization or bacterial decomposition into inorganic phosphorus before utilization by phytoplankton In their work on Lake Huron and Saginaw Bay, Di Toro and Matystik (1980) proposed a nutrient recycle formulation that was a function of the localized phytoplankton population This proposal was based on both an analysis of available field data and the work of others (Hendry 1977 Lowe, 1976, Henrici, 1938, Menon 1972, and Rao, 1976) that indicated bacterial biomass increased as phytoplankton biomass increased EUTRO5 uses a saturating recycle mechanism a compromise between conventional first-order kinetics and a second order recycle mechanism wherein the recycle rate is directly proportional to the phytoplankton biomass present, as had been indicated in pure culture, bacteria-seeded, laboratory studies (Jewell and McCarty, 1971)

Saturating recycle permits second order dependency at low phytoplankton concentrations, when $P_c << K_{mPc}$, where K_{mPc} is the half-saturation constant for recycle, and permits first order recycle when the phytoplankton greatly exceed the half-saturation constant Basically this mechanism slows the recycle rate if the phytoplankton population is small, but does not permit the rate to increase continuously as phytoplankton increase The assumption is that at higher population levels, recycle kinetics proceed at the maximum first order rate The default value for K_{mPc} is 0, which causes mineralization to proceed at its first order rate at all phytoplankton levels

Sorption

There is an adsorption-desorption interaction between dissolved inorganic phosphorus and suspended particulate matter in the water column The subsequent settling of the suspended solids together with the sorbed inorganic phosphorus can act as a significant loss mechanism in the water column and is a source of phosphorus to the sediment Because the rates of reaction for adsorption-desorption are in the order of minutes versus reaction rates in the order of days for the biological kinetics, an equilibrium assumption can be made This equilibrium reaction implies that the dissolved and particulate phosphorus phases instantaneously react to any discharge sources of phosphorus or runoff or shoreline erosion of solids so as to redistribute the phosphorus to its "equilibrium" dissolved and solids phase concentrations

Consider C_{DIP} to be the concentration of dissolved inorganic phosphorus in the water column It interacts with the particulate concentration, C_{PIP} The interaction may be an adsorption-desorption process with the solids or an assimilation-depuration process with the phytoplankton If the total suspended solids is considered the particulate concentration can be defined as

$$C_{PIP} = C_{PIP}\,M \qquad 5\ 16$$

where

C_{PIP} = concentration of phosphorus sorbed to solids, mg P/kg M

M = concentration of solids, kg/L

The total inorganic phosphorus is then the sum of dissolved inorganic and the particulate inorganic phosphorus

$$C_3 = C_{DIP} + C_{PIP} \qquad 5\ 17$$

The underlying assumption that is made, as mentioned previously, is "instantaneous equilibrium" between the adsorption-desorption processes The equilibrium between the dissolved inorganic phosphorus in the water column and the mass concentration of inorganic phosphorus of the solids is usually expressed in terms of a partition coefficient

$$K_{PIP} = \frac{C'_{PIP}}{C_{DIP}} \qquad 5\ 18$$

where

K_{PIP} = partition coefficient for particulate phosphorus (mg P/kg M) per (mg P/L) or (L/kg M)

Substituting equation 5 18 into 5 16 gives

$$C_{PIP} = K_{PIP}\,M\,C_{DIP} \qquad 5\ 19$$

Equation 5 19 is the linear portion of the Langmuir isotherm Although not always representative of actual conditions, it is a reasonable approximation when the sorbed phosphorus concentration is much less than the ultimate adsorbing capacity of the solids Combining Equations 5 17 and 5 19, the total concentration may be expressed as

$$C_3 = C_{DIP} + K_{PIP}\, M\, C_{DIP} \tag{5 20}$$

The dissolved and particulate fractions may be expressed, respectively, as

$$f_{D3} = \frac{C_{DIP}}{C_3} = \frac{1}{1 + K_{PIP}\, M} \tag{5 21}$$

$$f_{P3} = \frac{C_{PIP}}{C_3} = \frac{K_{PIP}\, M}{1 + K_{PIP}\, M} \tag{5 22}$$

A wide range of partition coefficients is found in the literature Thomann and Fitzpatrick (1982) report values between 1,000 and 16,000 Using a range in partition coefficients from 1 000 - 16 000 and a range of inorganic solids of from 10 to 30 mg/L in the water column leads to a range in the fraction particulate inorganic phosphorus of from 0 01 to 0 33 In EUTRO5, the dissolved and particulate phosphorus phases are assigned as spatially-variable, time-constant fractions of the total inorganic phosphorus

$$C_{DIP\ i} = f_{D3i}\, C_{3i} \tag{5 23}$$

$$C_{PIP\ i} = (1 - f_{D3i})\ C_{3i} \tag{5 24}$$

where

C_{3i} = the total inorganic phosphorus in segment i, mg/L

4. PHYTOPLANKTON NITROGEN

$$\frac{\partial (C_4 a_{NC})}{\partial t} = \underbrace{G_{P1} a_{NC} C_4}_{growth} - \underbrace{D_{P1} a_{NC} C_4}_{death} - \underbrace{\frac{v_{s4}}{D} a_{NC} C_4}_{settling}$$

8. ORGANIC NITROGEN

$$\frac{\partial C_7}{\partial t} = \underbrace{D_{P1} a_{NC} f_{ON} C_4}_{death} - \underbrace{k_{71} \theta_{71}^{T-20} \left(\frac{C_4}{K_{mPc} + C_4} \right) C_7}_{mineralization} - \underbrace{\frac{v_{s3} (1 - f_{D7})}{D} C_7}_{settling}$$

3. AMMONIA NITROGEN

$$\frac{\partial C_1}{\partial t} = \underbrace{D_{P1} a_{NC} (1 - f_{ON}) C_4}_{death} + \underbrace{k_{71} \theta_{71}^{T-20} \left(\frac{C_4}{K_{mPc} + C_4} \right) C_7}_{mineralization} - \underbrace{G_{P1} a_{NC} P_{NH3} C_4}_{growth} - \underbrace{k_{12} \theta_{12}^{T-20} \left(\frac{C_6}{K_{NIT} + C_6} \right) C_1}_{nitrification}$$

2. NITRATE NITROGEN

$$\frac{\partial C_2}{\partial t} = \underbrace{k_{12} \theta_{12}^{T-20} \left(\frac{C_6}{K_{NIT} + C_6} \right) C_1}_{nitrification} - \underbrace{G_{P1} a_{NC} (1 - P_{NH3}) C_4}_{growth} - \underbrace{k_{2D} \theta_{2D}^{T-20} \left(\frac{K_{NO3}}{K_{NO3} + C_4} \right) C_2}_{denitrification}$$

where

$$P_{NH3} = \underbrace{C_1 \left(\frac{C_2}{(K_{mN} + C_1)(K_{mN} + C_2)} \right) + C_1 \left(\frac{K_{mN}}{(C_1 + C_2)(K_{mN} + C_2)} \right)}_{ammonia\ preference\ factor}$$

Figure 5 5 Nitrogen cycle equations

f_{D3i} = the fraction of the total inorganic phosphorus assigned to the dissolved phase in segment i

$C_{DIP\ i}$ = the equilibrium dissolved inorganic phosphorus in segment i, available for algal uptake, mg/L

C_{PIP} = the equilibrium sorbed inorganic phosphorus in segment i which may then settle to the sediment layer from the water column, mg/L

Settling

Particulate organic and inorganic phosphorus settle according to user-specified velocities and particulate fractions Particulate organic phosphorus is equated to solid type 1, which represents organic matter Time and segment-variable organic matter settling velocities $v_{s3,i}$ can be input by the user using transport field 3 Segment-variable organic phosphorus dissolved fractions $f_{D8,i}$ are input with initial conditions

Particulate inorganic phosphorus is equated to solid type 3, which represents inorganic sediment Time and segment variable inorganic phosphorus settling velocities, $v_{s5,i}$ can be input by the user using transport field 5 Segment-variable inorganic phosphorus dissolved fractions, $f_{D3,i}$ are input with initial conditions

The Nitrogen Cycle

Four nitrogen variables are modeled phytoplankton nitrogen, organic nitrogen, ammonia, and nitrate A summary is illustrated in Figure 5 5 Table 5 6 summarizes the terms used in the nitrogen system kinetics

Phytoplankton Growth

As phytoplankton grow, dissolved inorganic nitrogen is taken up and incorporated into biomass For every mg of phytoplankton carbon produced, a_{NC} mg of inorganic nitrogen is taken up Both ammonia and nitrate are available for uptake and use in cell growth by phytoplankton however, for physiological reasons, the preferred form is ammonia nitrogen The ammonia preference term P_{N-3} is given in Figure 5 5

The behavior of this equation, for a Michaelis value, K_{mN},

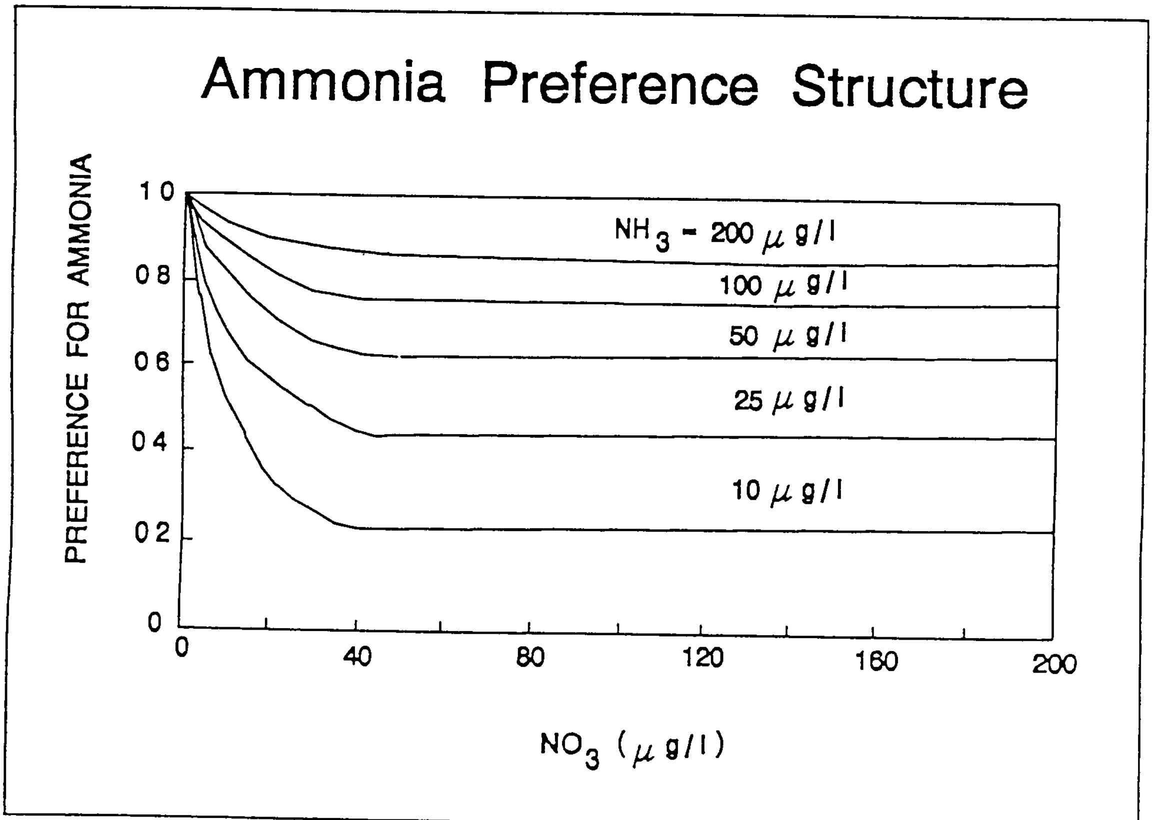


Figure 5 6 Ammonia preference structure (Thomann and Fitzpatrick, 12982)

Table 5 6 Nitrogen Reaction Terms

Description	Notation	Value from Potomac Estuary Model	Units	
Nitrogen to carbon ratio	a_{NC}	0 25	mg N/gm C	CNC23
Organic nitrogen mineralization rate @ 20蚓 °C	k_{71}	0 075	day ^{1}	K71C
Temperature coefficient	θ_{71}	1 08	-	K71T
Nitrification rate	k_{12}	0 09-0 13	day ^{1}	K12C
Temperature coefficient	θ_{12}	1 08	-	K12T
Half saturation constant for oxygen limitation of nitrification	K_{NIT}	2 0	mg O_2/L	KNIT
Denitrification rate at 20蚓	k_{2D}	0 09	day ^{1}	K20C
Temperature coefficient	θ_{2D}	1 045	-	K20T
Michaelis constant for denitrification	K_{NO3}	0 1	mg O_2/L	KNO3
Fraction of dead and respired phytoplankton recycled				FON
to the organic nitrogen pool	f_{ON}	0 5	-	
to the ammonia nitrogen pool	$(1-f_{ON})$	0 5	-	
Preference for ammonia uptake term	P_{NH3}	eq 5 30	-	
Fraction dissolved organic nitrogen	f_{D7}	1 0	-	
Organic matter settling velocity	v_{s3}	-	m/day	

of 25 痢 N/L, is shown in Figure 5 6 The behavior of this equation is most sensitive at low values of ammonia or nitrate For a given concentration of ammonia, as the available nitrate

increases above approximately the Michaelis limitation, the preference for ammonia reaches an asymptote Also as the concentration of available ammonia increases, the plateau level off at values closer to unity, i e , total preference for ammonia

Phytoplankton Death

As phytoplankton respire and die, living organic material recycled to nonliving organic and inorganic matter For every m of phytoplankton carbon consumed or lost, a_{NC} mg of nitrogen is released During phytoplankton respiration and death, a fractio of the cellular nitrogen f_{on} is organic while $(1 - f_{on})$ is in th inorganic form of ammonia nitrogen The fraction recycled to th inorganic pool for Great Lakes models has been assigned at 50% (Di Toro and Matystik, 1980)

Mineralization

Nonliving organic nitrogen must undergo mineralization or bacterial decomposition into ammonia nitrogen before utilization by phytoplankton In EUTRO5, the first order, temperature-corrected rate constant is modified by a saturated recycle term as explained in the phosphorus mineralization section This mechanism slows the mineralization rate if the phytoplankton population is small, but does not permit the rate to increase continuously as phytoplankton increase The default value for the half-saturation constant K_{mPc} is 0 which causes mineralization to proceed at its first order rate at all phytoplankton levels

Settling

Particulate organic nitrogen settles according to user-specified velocities and particulate fractions Particulate organic nitrogen is equated to solid type 1 which represents organic matter Time and segment-variable organic matter settling velocities v_{s3} can be input by the user using transport field 3 Segment-variable organic nitrogen dissolved fractions, f_{D7}, are input with initial conditions

Nitrification

Ammonia nitrogen in the presence of nitrifying bacteria and oxygen is converted to nitrate nitrogen (nitrification) The process of nitrification in natural waters is carried out by aerobic autotrophs Nitrosomonas and Nitrobacter predominate in fresh waters It is a two-step process with Nitrosomonas bacteria responsible for the conversion of ammonia to nitrite and Nitrobacter responsible for the conversion of nitrite to nitrate

Essential to this reaction process are aerobic conditions Also this process appears to be affected by high or low values of pH that inhibit Nitrosomonas growth, particularly for pH below 7 and greater than 9 As with phytoplankton, the nitrifying bacterial populations are sensitive to flow During periods of high flow or storm runoff upstream bacteria may be advected downstream, with some lag time after a flow transient before they can build up to significant levels again

The process of nitrification in natural waters, then, is complex, depending on dissolved oxygen, pH, and flow conditions, which in turn leads to spatially and temporally varying rates of nitrification To properly account for this complex phenomenon in the modeling framework would be difficult and would require a data base that is usually unavailable

The kinetic expression for nitrification in EUTRO5 contains three terms -- a first order rate constant, a temperature correction term, and a low DO correction term The first two terms are standard The third term represents the decline of the nitrification rate as DO levels approach 0 The user may specify the half-saturation constant K_{NIT}, which represents the DO level at which the nitrification rate is reduced by half The default value is zero, which allows this reaction to proceed fully even under anaerobic conditions

Denitrification

Denitrification refers to the reduction of NO_3 (or NO_2) to N_2 and other gaseous products such as N_2O and NO This process is carried out by a large number of heterotrophic, facultative anaerobes Under normal aerobic conditions found in the water column, these organisms use oxygen to oxidize organic material Under the anaerobic conditions found in the sediment bed or during extremely low oxygen conditions in the water column however, these organisms are able to use NO_3 as the electron acceptor

The process of denitrification is included in the modeling framework simply as a sink of nitrate The kinetic expression for denitrification in EUTRO5 contains three terms -- a first order rate constant, a temperature correction term, and a DO correction term The first two terms are standard The third term represents the decline of the denitrification rate as DO levels rise above 0 The user may specify the half-saturation constant K_{NO3}, which represents the DO level at which the denitrification rate is reduced by half The default value is zero which prevents this reaction at all DO levels Denitrification is assumed to always occur in the sediment layer where anaerobic conditions always exist

The Dissolved Oxygen Balance

Five state variables participate in the DO balance phytoplankton carbon ammonia, nitrate carbonaceous biochemical oxygen demand, and dissolved oxygen A summary is illustrated in Figure 4 2 The reduction of dissolved oxygen is a consequence of the aerobic respiratory processes in the water column and the anaerobic processes in the underlying sediments Both these processes contribute significantly and, therefore, it is necessary to formulate their kinetics explicitly

The dissolved oxygen processes in EUTRO5 are discussed in Chapter 4 The CBOD and DO reaction terms are summarized in Table 4 1

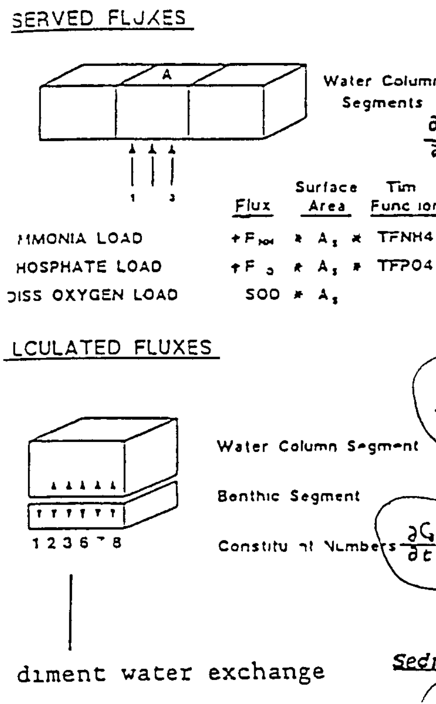
Benthic - Water Column Interactions

The decomposition of organic material in benthic sediment can have profound effects on the concentrations of oxygen and nutrients in the overlying waters The decomposition of organic material releases nutrients to the sediment interstitial waters and also results in the exertion of an oxygen demand at the sediment-water interface As a result, the areal fluxes from the sediment can be substantial nutrient sources or oxygen sinks to the overlying water column Additionally, the occurrence of anoxia, due in part to the sediment oxygen demand, may dramatically increase certain nutrient fluxes through a set of complex redox reactions that change the state and concentrations of various nutrients and metals thereby releasing bound nutrients The relative importance of the sediment oxygen demand and nutrient fluxes vis-a-vis future nutrient control strategies requires the incorporation of a dynamic sediment layer and its associated interactions with the overlying water column in a framework that is consistent with that discussed in the previous sections

EUTRO5 provides two options for nutrient and oxygen fluxes descriptive input and predictive calculations (Fig 5 8) The first option is used for networks composed of water column segments only Spatially-variable observed fluxes must be specified for ammonia phosphate and sediment oxygen demand Time functions may be specified for ammonia and phosphate, reflecting seasonal changes Seasonal changes in water temperature can affect SOD through its temperature coefficient

Benthic Simulation

The calculational framework incorporated for benthic-water column exchange draws principally from a study of Lake Erie, which incorporated sediment-water column interactions performed by Di Toro and Connolly (1980) For a surficial benthic layer



A ORGANIC NITROGEN

$$\frac{\partial C_7}{\partial t} = k_{PED}\theta_{PED}^{T-20} a_{nc} f_{on} C - k_{OMD}\theta_{OMD}^{T-20} C_7$$

algal decomposition mineralization

1. AMMONIA NITROGEN

$$\frac{\partial C_1}{\partial t} = k_{PZD}\theta^{T-20} a_{nc} (1 - f_{on}) C_4 + k_{OMD}\theta_{OMD}^{T-20} C_1$$

algal decomposition mineralization

2. NITRATE NITROGEN

$$\frac{\partial C_2}{\partial t} = - k_{2D}\theta_{2D}^{T-20} C_2$$

denitrification

B. ORGANIC PHOSPHORUS

$$\frac{\partial C_8}{\partial t} = k_{PED}\theta_{PED}^{T-20} a_{PC} f_{op} C_4 - k_{OPD}\theta_{OPD}^{T-20} f_{D8} C_8$$

algal decomposition mineralization

3. INORGANIC PHOSPHORUS

$$\frac{\partial C_3}{\partial t} = k_{PED}\theta_{PED}^{T-20} a_{pc} (1 - f_{op}) C_4 + k_{OPD}\theta_{OPD}^{T-20} f_{D8} C_8$$

algal decomposition mineralization

Figure 5 9 Benthic nutrient equations

Sediment Flux for Chemical K (g/m²-day)

$$FLUX = \frac{E_{DIF}}{D_j} (C_{Kj} f_{Kj} - C_{Ki} f_{Ki})$$

(*for benthic segment j water segment i*)

Figure 5 8 Sediment-water exchange

with thickness D_j, the nitrogen and phosphorus mass balance equations are summarized in Figure 5 9 and Table 5 7 The benthic CBOD and DO equations were summarized in Figure 4 3 and Table 4 2 in the previous chapter

WASP5 allows a more detailed parameterization of settling into the benthos that includes not only a downward settling velocity but an upward resuspension velocity as well In this context then the net particulate flux to the sediment is due to the difference between the downward settling flux and the upward resuspension flux

Benthic Depth -- One of the first decisions to be made regarding the benthic layer is to determine its depth Two factors influence this decision The first is to adequately reflect the thickness of the active layer, the depth to which the sediment is influenced by exchange with the overlying water column Secondly one wishes the model to reflect a reasonable time history or memory' in the sediment layer Too thin a

[illegible]

Description	Notation	Value from Potomac Estuary Study	Units
Anaerobic algal decomposition rate	k_{PZD} KPZDC 55	0 02	day ^{1}
Temperature coefficient	θ_{PZD} KPZDT 56	1 08	none
Organic nitrogen decomposition rate	k_{OND} KONDC	0 0004	day ^{1}
Temperature coefficient	θ_{OND} KONDT	1 08	none
Organic phosphorus decomposition rate	k_{OPD} KOPDC	0 0004	day ^{1}
Temperature coefficient	θ_{OPD} KOPDT	1 08	none
Fraction inorganic phosphorus dissolved in benthic layer	f_{D3j}	0 045-0 001	none
Diffusive exchange coefficient	E_{DIF}	2-2 5 x 10^{4}	m^2/day
Benthic layer depth	D_j	0 1-0 3	m
Benthic layer	j		
Water column	i		

layer and the benthos will 'remember or be influenced by deposition of material that would have occurred only within the last year or two of the period being analyzed, too thick a layer and the model will "average too long a history, not reflecting, as in the case of phosphorus substantial reductions in sedimentary phosphorus resulting from reduced phosphorus discharges from sewage treatment plants The choice of sediment thickness is further complicated by spatially variable sedimentation rates The benthic layer depths, together with the assigned sedimentation velocities provide for a multi-year detention time or memory', providing a reasonable approximation of the active layer in light of the observed pore water gradients

Benthic Nitrogen -- The next consideration is the application of these mass balance equations to the nitrogen species in a reducing sediment (Berner 1974) Particulate organic nitrogen is hydrolyzed to ammonia by bacterial action within the benthos In addition to the ammonia produced by the hydrolysis of particulate organic nitrogen in the benthos ammonia is generated by the anaerobic decomposition of algae I a study of this reaction, Foree and McCarty (1970) showed that the anaerobic rate of decay of algae is substantial (0 007-0 022 day^{-1}) However, the end product initially is not exclusively ammonia Rather, a fraction of the algal nitrogen becomes particulate organic nitrogen, which must undergo hydrolysis before becoming ammonia

Ammonia produced by the hydrolysis of non-algal organic nitrogen and the decomposition of detrital algal nitrogen may then be exchanged with the overlying water column via diffusion No nitrification occurs in the sediment due to the anaerobic conditions present in the sediment Denitrification, the conversion of nitrate to nitrogen gas, may occur however Nitrate is present in the benthos due to diffusive exchange with the overlying water column

The analysis of the benthic nitrogen concentrations and the resulting flux of ammonia is relatively straightforward because of the simplicity of the kinetics hydrolysis and anaerobic algal decay produce a stable end product, ammonia, which does not undergo further reactions in the anaerobic sediment The equations resulting from the above framework are presented in Figure 5 9, and the coefficients are summarized in Table 5 7

Benthic Phosphorus -- A complete analysis of the phosphorus fluxes from sediments would require a rather complex and elaborate computation of solute-precipitate chemistry and its interaction with the mass transport of the dissolved species The reasons for this are twofold first, it is well known (Nriagu, 1972) that for phosphorus the formation of precipitates affects the interstitial water concentrations, thereby affecting the interstitial water transport of the various phosphorus forms or species second, the dissolved concentrations are affected by the redox reactions, which in turn, affect the phosphorus fluxes that occur during aerobic and anaerobic conditions (Phosphorus fluxes are enhanced under anaerobic conditions)

A computation of solute-precipitate chemistry was judged to be outside the scope of this model Instead a simplified approach was taken, which to a large degree relies on empiricism Anaerobic decomposition of detrital algal phosphorus is assumed to occur using the same rate expressions and rate constants as those for detrital algal nitrogen, yielding both organic and inorganic phosphorus Anaerobic decomposition of organic phosphorus then proceeds A spatially-variable fraction of the end product, dissolved inorganic phosphorus remains in the interstitial water and is not involved in the formation of precipitates and is not sorbed onto the benthic solids This spatial variation reflects the ionic chemical makeup of the benthos in various regions of the water body

Using observed total and interstitial dissolved inorganic phosphorus values, the fraction dissolved inorganic phosphorus can be assigned to each segment, with the particulate and dissolved inorganic phosphorus computed for each time step in a manner similar to the overlying water column inorganic phosphorus (equations 5 25 through 5 27) Exchange of the dissolved phosphorus forms with the overlying water column is also similar to that of ammonia, nitrate, and dissolved oxygen Mass flux equations are presented in Figure 5 9 The effects of anoxia upon sediment phosphorus flux were not included in the modeling framework The approach used to generate sediment phosphorus flux, although not entirely satisfactory, is at least consistent with the framework within which the fluxes of other materials are being generated

Benthic Carbon -- The reactions that convert algal and refractory carbon to their end products are complex The initial step in which the algal and refractory carbon are converted to reactive intermediates appears to be similar to the refractory organic and algal nitrogen degradation, and in the subsequent calculations the rates for carbon and nitrogen decomposition are assumed to be equal The reactive intermediates, however participate in further reactions for example, volatile acids react to become methane, and the mechanisms that control these reactions are somewhat uncertain In addition few measurements of these intermediate species are available and a calculation that incorporates their concentrations explicitly would of necessity be speculative Thus one uses a simplified, yet realistic, formulation of these reactions

The method proposed by Di Toro and Connolly (1980), and highlighted here is based upon separating the initial reactions that convert sedimentary organic material into reactive intermediates and the remaining redox reactions that occur Then using a transformation variable and an orthogonality relationship, Di Toro and Connolly derive mass balance equations that are independent of the details of the redox equations Rather they are only functions of the component concentration and it suffices to compute only the component concentrations, which can be treated in exactly the same way as any other variable in the mass transport calculation

The convenient choice of components for the calculation are those that parallel the aqueous variables -- carbonaceous BOD and dissolved oxygen Restricting the calculation to these components, however, eliminates the possibility of explicitly including the effects of other reduced species such as iron, manganese and sulfide, which play a role in overall redox reactions and may be involved in the generation of sediment oxygen demand This simplification appears reasonable in light of the preliminary nature of the benthic calculation

The decomposition reactions that drive the component mass balance equations are the anaerobic decomposition of the algal carbon, and the anaerobic breakdown of the benthic organic carbon Both reactions are sinks of the oxygen and rapidly drive its concentration negative, indicating that the sediment is reduced rather than oxidized The negative concentrations computed can be considered the oxygen equivalents of the reduced end products produced by the chains of redox reactions occurring in the sediment

Because the calculated concentration of oxygen is positive in the overlying water, it is assumed that the reduced carbon species (negative oxygen equivalents) that are transported across the benthic water interface combine with the available oxygen and are oxidized to CO_2 and H_2O with a consequent reduction of oxygen in the overlying water column The sediment mass balance equations for carbonaceous BOD and DO, together with the equation for sediment oxygen demand, are presented in Figure 4 3 and Table 4 2

5 2 MODEL IMPLEMENTATION

To simulate eutrophication with WASP5, use the preprocessor to create a EUTRO5 input dataset For the portions of the dataset describing environment, transport, and boundaries, EUTRO5 model input will be similar to that for the conservative tracer model as described in Chapter 2 To those basic parameters, the user will add combinations of transformation parameters and perhaps solids transport rates

EUTRO5 kinetics can be implemented using some or all of the processes and kinetic terms described above to analyze eutrophication problems For convenience three levels of complexity are identified here (1) simple eutrophication kinetics, (2) intermediate eutrophication kinetics, and (3) intermediate eutrophication kinetics with benthos Please note that the discrete levels of simulation identified here are among a continuum of levels that the user could implement

The three implementation levels are described briefly below, along with the input parameters required to solve the eutrophication equations in EUTRO5 Input parameters are prepared for WASP5 in four major sections of the preprocessor -- environment, transport boundaries and transformation Basic model parameters are described in Chapter 2 and will not be repeated here The eight state variables with abbreviations used in this text are listed in Table 5 8

Table 5 8 Summary of EUTRO5 Variables

	Variable	Notation	Concentration	Units
1	Ammonia Nitrogen	NH3	C_1	mg N/L
2	Nitrate Nitrogen	NO3	C_2	mg N/L
3	Inorganic Phosphorus	PO4	C_3	mg P/L
4	Phytoplankton Carbon	PHYT	C_4	mg C/L
5	Carbonaceous BOD	CBOD	C_5	mg O_2/L
6	Dissolved Oxygen	DO	C_6	mg O_2/L
7	Organic Nitrogen	ON	C_7	mg N/L
8	Organic Phosphorus	OP	C_8	mg P/L

Simple Eutrophication Kinetics

Simple eutrophication kinetics simulate the growth and death of phytoplankton interacting with one of the nutrient cycles Growth can be limited by the availability of inorganic nitrogen or inorganic phosphorus, and light Equations include phytoplankton kinetics

$$S_{k4} = \left(G_{P1} - D_{P1} - \frac{v_{84}}{D}\right) C_4 \qquad 5\ 25$$

and either the phosphorus cycle

$$S_{k8} = +D_{P1} a_{PC} C_4 - k_{83} \theta_{83}^{T-20} C_8 - \frac{v_{83}}{D} (1 - f_{D8}) C_8 \qquad 5\ 26$$

$$S_{k3} = +k_{83}\theta_{83}^{T-20}C_8 - G_{P1}a_{PC}C_4 - \frac{V_{B5}}{D}(1-f_{D3})\,C_3 \qquad 5.27$$

or the nitrogen cycle

$$S_{k7} = +D_{P1}a_{NC}C_4 - k_{71}\theta_{71}^{T-20}C_7 - \frac{V_{B3}}{D}(1-f_{D7})\,C_7 \qquad 5.28$$

$$S_{k1} = +k_{71}\theta_{71}^{T-20}C_7 - G_{P1}a_{PC}P_{NH_3}C_4 - k_{12}\theta_{12}^{T-20}C_1 \qquad 5.29$$

$$S_{k2} = +k_{12}\theta_{12}^{T-20}C_1 - G_{P1}a_{NC}(1-P_{NH_3})\,C_4 \qquad 5.30$$

where S_{ki} is the source/sink term for variable "i" in a segment, in mg/L-day. Kinetic rate constants and coefficients are as defined in Tables 5.3, 5.5, and 5.6.

Phytoplankton plus either three nitrogen variables or two phosphorus variables are used in simple eutrophication simulations. While phytoplankton are simulated internally as mg/L carbon, initial concentrations and boundary concentrations are input by the user as µg/L chlorophyll *a*. EUTRO5 converts these input concentrations to internal concentrations using a user-specified carbon to chlorophyll ratio. If the carbon to chlorophyll ratio is not input, then a default value of 30 is used. Internal concentrations of phytoplankton nitrogen and phytoplankton phosphorus are calculated from user-specified nitrogen to carbon and phosphorus to carbon ratios. If these ratios are not input, then default values of 0.25 and 0.025 are used.

Simple eutrophication kinetics assume that death returns phytoplankton nitrogen and phosphorus entirely to the organic nitrogen and organic phosphorus pools. Mineralization is a simple first order function that is unaffected by phytoplankton levels, and nitrification is a simple first order function unaffected by dissolved oxygen. Denitrification is not simulated

Light limitation is described by the Di Toro formulation equation 5 4, and the user must calibrate the saturating light intensity I_s

The particulate fractions of ON and OP are associated with transport field 3, organic matter settling Particulate PHYT i associated with transport field 4 The particulate fraction of PO4 is associated with transport field 5, inorganic settling

Environment Parameters

These parameters define the basic model identity, including the segmentation, and control the simulation

Systems-- Select 'simulate for PHYT and either ON NH3, and NO3, or OP and PO4 Select "constant for the nonsimulated nutrients and 'bypass for CBOD and DO During calibration, the user may select 'constant" or "bypass" for any selected variables (Group A Record 4 NOSYS Record 9, SYSBY)

Segments-- Water column segments should be defined in the standard fashion If settling is to be simulated (i e for ON OP PHYT or PO4) the user should add a single benthic segment underlying all water column segments This benthic segment will merely act as a convenient sink for settling organic matter Model calculations within this benthic segment should be ignored (Group A, Record 4, NOSEG, Group C, Record 3, ISEG, IBOTSG, ITYPE BVOL, DMULT)

Transport Parameters

This group of parameters defines the advective and dispersive transport of model variables

Number of Flow Fields-- To simulate settling of ON and OP the user should select solids 1 flow under advection To simulate settling of PHYT the user should select solids 2 flow To simulate PO4 settling, the user should select solids 3 flow The user should also select water column flow (Group D, Record 1 NFIELD)

Particulate Transport, m^3/sec-- Time variable settling and resuspension rates for solids 1 solids 2, and solids 3 can be input using the continuity array BQ and the time function QT For each solids flow field, cross-sectional exchange areas (m^2) for adjacent segment pairs are input using the spatially-variable BQ Time-variable settling velocities can be specified as a series of velocities in m/sec, versus time If the units conversion factor is set to 1 157e-5, then these velocities are input in units of m/day. These velocities are multiplied internally by cross-sectional areas and treated as flows that carry particulate organic matter out of the water column. (Group D, Record 4, BQ, JQ, IQ; Record 6, QT, TQ)

Boundary Parameters

This group of parameters includes boundary concentrations, waste loads, and initial conditions. Boundary concentrations must be specified for any segment receiving flow inputs, outputs, or exchanges. Initial conditions include not only initial concentrations, but also the density and solids transport field for each solid, and the dissolved fraction in each segment.

Boundary Concentrations, mg/L-- At each segment boundary, time variable concentrations must be specified for PHYT, expressed as µg/L chlorophyll *a*. Time variable concentrations must also be specified for either ON, NH3, and NO3, or OP and PO4. A boundary segment is characterized by water exchanges from outside the network, including tributary inflows, downstream outflows, and open water dispersive exchanges. (Group E, Record 4, BCT)

Waste Loads, kg/day-- For each point source discharge, time variable PHYT, ON, NH3, NO3, OP, and PO4 loads can be specified. These loads can represent municipal and industrial wastewater discharges, or urban and agricultural runoff. If any phytoplankton loads are specified, they should be in units of kg carbon/day. (Group F, Record 4, WKT)

Solids Transport Field-- The transport fields associated with particulate settling must be specified under initial conditions. Solids 1 (Field 3) is recommended for ON and OP. Solids 2 (Field 4) is recommended for PHYT. Solids 3 (Field 5) is recommended for PO4. (Group J, Record 1, IFIELD)

Solid Density, g/cm^3-- A value of 0 can be entered for the nominal density of PHYT, ON, NH3, NO3, OP and PO4. This information is not used in EUTRO5. (Group J, Record 1, DSED)

Initial Concentrations, mg/L-- Concentrations of PHYT, expressed as µg/L chlorophyll *a* and either ON, NH3, and NO3 or OP and PO4 in each segment must be specified for the time at which the simulation begins. For the nonsimulated nutrients held constant, average concentrations must be specified. These nutrient concentrations will remain constant throughout the simulation and can affect PHYT through growth rate limitation (although nonsimulated nutrients should be in excess and therefore not affect growth). Concentrations of zero for bypassed variables -- CBOD and DO -- will be entered by the preprocessor. (Group J, Record 2, C)

Dissolved Fraction-- The dissolved fraction of PHYT, ON, NH3, NO3, OP, and PO4 in each segment must be specified. The dissolved fraction of PHYT should be set to 0. Only the particulate fractions of the nutrients will be subject to settling. (Group J Record 2, DISSF)

Transformation Parameters

This group of parameters includes spatially variable parameters, constants, and kinetic time functions for the water quality constituents being simulated. Parameter values are entered for each segment. Specified values for constants apply over the entire network for the whole simulation. Kinetic time functions are composed of a series of values versus time, in days.

Water Temperature, C-- Time and segment variable water temperatures can be specified using the parameters TMPSG and TMPFN, and the time functions TEMP(1-4). If temperatures are to remain constant in time, then the user should enter segment temperatures using the parameter TMPSG. TMPFN and TEMP(1-4) should be omitted.

If the user wants to enter time-variable temperatures, then values for the parameter TMPSG should be set to 1.0. The parameter TMPFN indicates which temperature function will be used by the model for each segment. Values of 1.0, 2.0, 3.0 or 4.0 will call time functions TEMP(1), TEMP(2), TEMP(3), and TEMP(4), respectively. Water temperatures should then be entered via these time functions as a series of temperature versus time values. The product of TMPSG and the selected TEMP function will give the segment and time specific water temperatures used by EUTRO5.

TMPSG and TMPFN are identified in EUTRO5 as parameters 3 and 4, respectively. TEMP(1-4) are identified in EUTRO5 as time functions 1-4. (Group G, Record 4, PARAM(I,3), PARAM(I,4), Group I, Record 2, VALT(1-4,K))

Solar Radiation, langleys/day-- Time-variable solar radiation at the water surface can be described using time functions ITOT and FDAY. Seasonally-varying values of solar radiation at the surface can be entered using ITOT with a series of radiation versus time values. FDAY gives the seasonally-varying fraction of day that is daylight, entered as a series of fraction versus time values. Internally, EUTRO5 uses the quotient ITOT/FDAY for the average radiation intensity during daylight hours. (Group I, Record 2, VALT(5,K), VALT(6,K))

Light Extinction, m^{-1}-- Time and segment variable light extinction coefficients can be specified using the parameters

KESG and KEFN, and the time functions KE(1-5) If extinction coefficients are to remain constant in time, then the user should enter segment coefficients using the parameter KESG KEFN and KE(1-4) should be omitted

If the user wants to enter time-variable extinction coefficients, then values for the parameter KESG should be set to 1 0 The parameter KEFN indicates which light extinction function will be used by the model for each segment Values of 1 0 2 0, 3 0, 4 0, or 5 0 will call time functions KE(1), KE(2) KE(3), KE(4), and KE(5), respectively Light extinction coefficients should then be entered via these time functions as a series of coefficient versus time values The product of KESG and the selected KE function will give the segment and time specific light extinction coefficients used by EUTRO5

KESG and KEFN are identified in EUTRO5 as parameters 5 and 6, respectively KE(1-4) are identified in EUTRO5 as time functions 8-12 (Group G Record 4 ISC, PARAM(I,5), PARAM(I 6) Group I, Record 2, VALT(8-12,K))

Growth Rate, day^{-1}-- The maximum phytoplankton growth rate constant and temperature coefficient can be input using constants K1C and K1T, respectively (Group H, Record 4, CONST(41), CONST(42))

Carbon to Chlorophyll Ratio, mg C/mg Chl-- The average carbon to chlorophyll weight ratio in phytoplankton can be specified using constant CCHL A default value of 30 is provided for in EUTRO5 (Group H, Record 4 CONST(46))

Light Limitation-- Available light is specified using time functions describing seasonal light at the water surface and segment- and time-variable light extinction coefficents These are described above

The Di Toro light limitation option can be specified using a value of 1 0 for LGHTS The saturating light intensity can then be specified using constant IS1 Default values for LGHTS and IS1 are 1 and 300 respectively (Group H Record 4 CONST(43) CONST(47))

Respiration Rate, day^{-1}-- The average phytoplankton respiration rate constant and temperature coefficient can be input using constants K1RC and K1RT respectively (Group H Record 4, CONST(50) CONST(51))

Death Rate, day^{-1}-- The non-predatory phytoplankton death rate constant can be input using constant K1D No temperature dependance is assumed (Group H, Record 4 CONST(52))

Phosphorus to Carbon Ratio, mg P/mg C-- The average phosphorus to carbon weight ratio in phytoplankton can be specified using constant PCRB. The EUTRO5 default value for PCRB is 0.025. (Group H, Record 4, CONST(57))

Phosphorus Mineralization Rate, day^{-1}-- The mineralization rate constant and temperature coefficient for dissolved organic phosphorus can be specified using constants K83C and K83T, respectively. (Group H, Record 4, CONST(100), CONST(101))

Phosphorus Half-Saturation Constant, mg P/L-- The phosphorus half-saturation constant for phytoplankton growth can be specified using constant KMPG1. When inorganic phosphorus concentrations are at this level, the phytoplankton growth rate is reduced by half. (Group H, Record 4, CONST(49))

Nitrogen to Carbon Ratio, mg N/mg C-- The average nitrogen to carbon weight ratio in phytoplankton can be specified using constant NCRB. The EUTRO5 default value for NCRB is 0.25. (Group H, Record 4, CONST(58))

Nitrogen Mineralization Rate, day^{-1}-- The mineralization rate constant and temperature coefficient for dissolved organic nitrogen can be specified using constants K71C and K71T, respectively. (Group H, Record 4, CONST(91), CONST(92))

Nitrification Rate, day^{-1}-- The nitrification rate constant and temperature coefficient for dissolved ammonia nitrogen can be specified using constants K12C and K12T, respectively. (Group H, Record 4, CONST(11), CONST(12))

Nitrogen Half-Saturation Constant, mg N/L-- The nitrogen half-saturation constant for phytoplankton growth can be specified using constant KMNG1. When inorganic nitrogen concentrations are at this level, the phytoplankton growth rate is reduced by half. This parameter also affects ammonia preference P_{NH3} as outlined in Figures 5.5 and 5.6. When KMNG1 = 0, P_{NH3} = 1.0. When KMNG1 becomes very large, P_{NH3} approaches a value of $C_1/(C_1 + C_2)$. (Group H, Record 4, CONST(48))

Intermediate Eutrophication Kinetics

Intermediate eutrophication kinetics simulate the growth and death of phytoplankton interacting with the nitrogen and phosphorus cycles and the dissolved oxygen balance. Growth can be limited by the availability of inorganic nitrogen, inorganic phosphorus, and light.

Intermediate eutrophication kinetics add CBOD and DO equations as well as certain nonlinear terms and functions to the simple eutrophication kinetics described above The oxygen balance equations and kinetic parameters are summarized in Figure 4 2 and Table 4 1 The phosphorus cycle equations and kinetic parameters are summarized in Figure 5 4 and Table 5 5 The nitrogen cycle equations and parameters are summarized in Figure 5 5 and Table 5 6 Phytoplankton equations are presented throughout Section 5 2, with parameters summarized in Table 5 3

Light limitation can be described by either the Di Toro or the Smith formulation The Smith formulation implements equations 5 6 through 5 11 These equations predict the carbon to chlorophyll ratio based on the availability of light, then predict the saturating light intensity based on the carbon to chlorophyll ratio

Other terms included in the intermediate kinetics equations are the phytoplankton effect on mineralization of organic phosphorus and nitrogen, the dissolved oxygen limitation on nitrification, the denitrification reaction, and zooplankton grazing The nonlinear DO balance equations can become important in inhibiting nitrification and carbonaceous oxidation and in promoting denitrification where low DO concentrations occur

All eight state variables are simulated in intermediate eutrophication simulations During calibration of the model to observed data, however, the user may want to bypass certain variables or hold them constant Nutrients can be held at observed concentrations, for instance, while phytoplankton growth and death rates are calibrated

Environment Parameters

These parameters define the basic model identity, including the segmentation and control the simulation

Systems-- Select simulate for all variables During calibration, the user may select constant or "bypass for any selected variables (Group A Record 4 NOSYS Record 9 SYSBY)

Segments-- Water column segments should be defined in the standard fashion If settling is to be simulated (i e for ON OP, PHYT, PO4 or CBOD), the user should add a single benthic segment underlying all water column segments This benthic segment will merely act as a convenient sink for settling organic matter Model calculations within this benthic segment should be ignored (Group A, Record 4, NOSEG, Group C, Record 3, ISEG, IBOTSG, ITYPE, BVOL, DMULT)

Transport Parameters

This group of parameters defines the advective and dispersive transport of model variables

Number of Flow Fields-- To simulate settling of ON, OP, and CBOD, the user should select solids 1 flow under advection To simulate settling of PHYT, the user should select solids 2 flow To simulate PO4 settling, the user should select solids 3 flow The user should also select water column flow (Group D, Record 1, NFIELD)

Particulate Transport, m^3/sec-- Time variable settling and resuspension velocities can be specified for particulate ON OP CBOD, PHYT, and PO4, as described in the simple eutrophication section above

Boundary Parameters

This group of parameters includes boundary concentrations, waste loads, and initial conditions Boundary concentrations must be specified for any segment receiving flow inputs, outputs or exchanges Initial conditions include not only initial concentrations, but also the density and solids transport field for each solid, and the dissolved fraction in each segment

Boundary Concentrations, mg/L-- At each segment boundary, time variable concentrations must be specified for PHYT expressed as μg/L chlorophyll *a* Time variable concentrations must also be specified for either ON, NH3, NO3 OP, PO4 CBOD, and DO A boundary segment is characterized by water exchanges from outside the network including tributary inflows, downstream outflows and open water dispersive exchanges (Group E, Record 4 BCT)

Waste Loads, kg/day-- For each point source discharge, time variable PHYT ON NH3 NO3, OP PO4, CBOD, and DO loads can be specified These loads can represent municipal and industrial wastewater discharges or urban and agricultural runoff If any phytoplankton loads are specified, they should be in units of kg carbon/day (Group F, Record 4, WKT)

Solids Transport Field-- The transport fields associated with particulate settling must be specified under initial conditions Solids 1 (Field 3) is recommended for ON, OP and CBOD Solids 2 (Field 4) is recommended for PHYT Solids 3 (Field 5) is recommended for PO4 (Group J, Record 1, IFIELD)

Solid Density, g/cm^3-- A value of 0 can be entered for the nominal density of PHYT ON, NH3, NO3, OP PO4 CBOD, and DO This information is not used in EUTRO5 (Group J, Record 1 DSED)

Initial Concentrations, mg/L-- Concentrations of all variables in each segment must be specified for the time at which the simulation begins Concentrations of PHYT are expressed as µg/L chlorophyll a (Group J, Record 2 C)

Dissolved Fraction-- The dissolved fraction of each variable in each segment must be specified The dissolved fraction of PHYT should be set to 0, and the dissolved fraction of DO should be set to 1 Only the particulate fractions of CBOD and the nutrients will be subject to settling (Group J, Record 2 DISSF)

Transformation Parameters

This group of parameters includes spatially variable parameters, constants, and kinetic time functions for the water quality constituents being simulated Parameter values are entered for each segment Specified values for constants apply over the entire network for the whole simulation Kinetic time functions are composed of a series of values versus time, in days

Water Temperature, C-- Time and segment variable water temperatures can be specified using the parameters TMPSG and TMPFN, and the time functions TEMP(1-4), as described in the simple eutrophication section above

gc/cm^2 day

Solar Radiation, langleys/day-- Time-variable solar radiation at the water surface can be described using time functions ITOT and FDAY, as described in the simple eutrophication section above

Light Extinction, m^{-1}-- Time and segment variable light extinction coefficients can be specified using the parameters KESG and KEFN, and the time functions KE(1-5), as described in the simple eutrophication section above

Growth Rate, day^{-1}-- The maximum phytoplankton growth rate constant and temperature coefficient can be input using constants K1C and K1T, respectively (Group H, Record 4, CONST(41), CONST(42))

Carbon to Chlorophyll Ratio, mg C/mg Chl-- The average carbon to chlorophyll weight ratio in phytoplankton can be specified using constant CCHL A default value of 30 is provided for in EUTRO5 If the Smith light limitation option is chosen then CCHL will be variable, recalculated daily throughout the simulation (Group -, Record 4, CONST(46))

Light Limitation-- Available light is specified using time functions describing seasonal light at the water surface and segment- and time-variable light extinction coefficents These are described above

The Di Toro light limitation option can be specified using value of 1 0 for LGHTS The saturating light intensity, in langleys/day can then be specified using constant IS1 Default values for LGHTS and IS1 are 1 and 300, respectively (Group H Record 4 CONST(43), CONST(47))

The Smith light limitation option can be specified using a value of 2 0 for LGHTS Two other parameters must then be specified The maximum quantum yield constant, in mg C/mole photons, can be specified using constant PHIMX The chlorophyll extinction coefficient, in (mg chl a/m^3)^{1}m^{1}, can be specified using constant XKC Default values for PHIMX and XKC are 720 and 0 017, respectively (Group H, Record 4, CONST(43), CONST(44), CONST(45))

Nitrogen Half-Saturation Constant, mg N/L-- The nitrogen half-saturation constant for phytoplankton growth can be specified using constant KMNG1 When inorganic nitrogen concentrations are at this level the phytoplankton growth rate is reduced by half This parameter also affects ammonia preference P_{NH3} as outlined in Figures 5 5 and 5 6 When KMNG1 = 0 P_{NH3} = 1 0 When KMNG1 becomes very large, P_{NH3} approaches a value of $C_1/(C_1 + C_2)$ (Group H, Record 4, CONST(48))

Phosphorus Half-Saturation Constant, mg P/L-- The phosphorus half-saturation constant for phytoplankton growth can be specified using constant KMPG1 When inorganic phosphorus concentrations are at this level, the phytoplankton growth rate is reduced by half (Group H, Record 4, CONST(49))

Nutrient Limitation Option-- The nutrient limitation formulation can be specified using constant NUTLIM A value of 0 selects the minimum formulation, which is recommended A value of 1 0 selects the multiplicative formulation The default value is 0 (Group H, Record 4 CONST(54))

Respiration Rate, day^{1}-- The average phytoplankton endogenous respiration rate constant and temperature coefficient can be input using constants K1RC and K1RT respectively (Group H, Record 4, CONST(50), CONST(51))

Death Rate, day -- The non-predatory phytoplankton death rate constant can be input using constant K1D No temperature dependance is assumed (Group H, Record 4, CONST(52))

Grazing Rate, day^{1}-- Zooplankton grazing can be specified using parameter ZOOSC time function ZOO, and constant K1G Time- and segment-variable herbivorous zooplankton populations are described as the product of the time variable population ZOO in mg zooplankton C/L, and segment specific ratios ZOOSG The grazing rate per unit zooplankton population, in L/mg zooplankton C-day, can be input using constant K1G The resulting grazing rate constant for phytoplankton is the product of the variable zooplankton population and the unit grazing rate (Note that ZOO can also be expressed as cells/L if K1G is expressed as L/cell-day) (Group G, Record 4, PARAM(I,15), Group H, Record 4, CONST(53), Group I, Record 2 VALT(19,K))

<u>Phosphorus to Carbon Ratio, mg P/mg C</u>-- The average phosphorus to carbon weight ratio in phytoplankton can be specified using constant PCRB The EUTRO5 default value for PCRB is 0 025 (Group H, Record 4, CONST(57)

<u>Phytoplankton Phosphorus Recycle</u>-- The fraction of dead and respired phytoplankton phosphorus that is recycled to the organic phosphorus pool can be specified using constant FOP The default value is 1 The fraction of phytoplankton phosphorus recycled directly to inorganic phosphorus is 1 - FOP (Group H, Record 4 CONST(104))

<u>Phosphorus Mineralization Rate, day^{-1}</u>-- The mineralization rate constant and temperature coefficient for dissolved organic phosphorus can be specified using constants K83C and K83T, respectively Phytoplankton effects on mineralization can be described using constant KMPHY, the half-saturation constant for mineralization dependence on phytoplankton, in mg C/L This causes mineralization rates to increase as phytoplankton levels increase If KMPHY is zero there is no phytoplankton effect on mineralization If KMPHY is large, then large concentrations of phytoplankton are needed to drive mineralization, and thus relatively low phytoplankton levels can lead to low mineralization rates (Group H, Record 4, CONST(100), CONST(101), CONST(59))

<u>Benthic Phosphorus Flux, mg/m^2-day</u>-- The segment- and time-variable benthic phosphorus flux can be specified using parameter FPO4 and time function TFPO4 The product of the spatially-variable FPO4 and time-variable TFPO4 gives the segment and time specific benthic flux for PO4 used by EUTRO5 Flux versus time values can be entered using TFPO4 while unitless segment ratios can be entered using FPO4 Values should be entered for water column segments that are in contact with the bottom of the water body (Group G, Record 4, PARAM(I,8) Group I, Record 2 VALT(14,K))

<u>Nitrogen to Carbon Ratio, mg N/mg C</u>-- The average nitrogen to carbon weight ratio in phytoplankton can be specified using constant NCRB The EUTRO5 default value for NCRB is 0 25 (Group H, Record 4, CONST(58)

<u>Phytoplankton Nitrogen Recycle</u>-- The fraction of dead and

respired phytoplankton nitrogen that is recycled to the organic nitrogen pool can be specified using constant FON The default value is 1 The fraction of phytoplankton nitrogen recycled directly to ammonia is 1 - FON (Group H Record 4 CONST(95))

Nitrogen Mineralization Rate, day^{-1}-- The mineralization rate constant and temperature coefficient for dissolved organic nitrogen can be specified using constants K71C and K71T, respectively Phytoplankton effects on mineralization can be described using constant KMPHY, the half-saturation constant for mineralization dependence on phytoplankton, as explained above in the phosphorus mineralization section (Group H, Record 4, CONST(91), CONST(92), CONST(59))

Nitrification Rate, day^{-1}-- The nitrification rate constant and temperature coefficient for dissolved ammonia nitrogen can be specified using constants K12C and K12T, respectively The half-saturation constant for oxygen limitation of nitrification can be specified using constant KNIT The default value for KNIT is 0 0, indicating no oxygen limitation (Group H, Record 4, CONST(11), CONST(12) CONST(13))

Denitrification Rate, day^{-1}-- The denitrification rate constant and temperature coefficient for dissolved nitrate nitrogen can be specified using constants K20C and K20T, respectively The half-saturation constant for oxygen limitation of denitrification can be specified using constant KNO3 The default value for KNO3 is 0 0, indicating no denitrification at oxygen concentrations above 0 0 (Group H, Record 4, CONST(21), CONST(22), CONST(23))

Benthic Nitrogen Flux, mg/m^2-day-- The segment- and time-variable benthic nitrogen flux can be specified using parameter FNH4 and time function TFNH4 The product of the spatially-variable FNH4 and time-variable TFNH4 gives the segment and time specific benthic flux for NH3 used by EUTRO5 Flux versus time values can be entered using TFNH4, while unitless segment ratios can be entered using FNH4 Values should be entered for water column segments that are in contact with the bottom of the water body (Group G, Record 4, PARAM(I,7) Group I, Record 2, VALT(13,K))

Sediment Oxygen Demand, g/m^2-day-- Segment variable sediment oxygen demand fluxes and temperature coefficients can be specified using the parameters SOD1D and SODTA respectively Values should be entered for water column segments that are in contact with the bottom of the water body (Group G, Record 4, PARAM(I,9), PARAM(I,12))

Reaeration Rate, day^{-1}-- There are three basic options for specifying reaeration -- a single rate constant segment and time variable rate constants, and flow and wind calculated rate constants. These options are described in Section 4.2, under the Streeter-Phelps transformation parameters.

CBOD Deoxygenation Rate, day^{-1}-- The CBOD deoxygenation rate constant and temperature coefficient can be specified using constants KDC and KDT, respectively. The half-saturation constant for oxygen limitation of carbonaceous deoxygenation can be specified using constant KBOD. The default value for KBOD is 0.0, indicating no oxygen limitation. (Group H, Record 4, CONST(72), CONST(73), CONST(75))

Intermediate Eutrophication Kinetics with Benthos

Simulating benthic interactions requires the addition of benthic segments to the model network. All state variables are simulated in the benthic segments. Dissolved fractions of NH3, NO3, PO4, CBOD, DO, ON, and OP may exchange with the water column by diffusion. Particulate fractions of PHYT, PO4, CBOD, ON, and OP may deposit to or be scoured from the benthic segments. Benthic layer decomposition rates for OP, ON, PHYT, and CBOD must be specified. The equations used are those presented in Figures 4.3 and 5.9. Rate parameters are summarized in Tables 4.2 and 5.7.

Many of the environment, transport, boundary, and transformation parameters required to implement this option are the same as those in the intermediate eutrophication option presented above. The benthic nitrogen and phosphorus flux functions should be omitted, and the following should be modified or added:

Segments-- Water column segments should be defined in the standard fashion. In addition, the user should add a benthic segment underlying each water column segment (or stack of water column segments). These benthic segments will receive settling organic and inorganic matter from the water column above, and can return material to the water column via resuspension or by pore water diffusion. (Group A, Record 4, NOSEG; Group C, Record 3, ISEG, IBOTSG, ITYPE, BVOL, DMULT)

Phytoplankton Decomposition, day^{-1}-- The user may specify the rate constant and temperature coefficient for phytoplankton decomposition in benthic segments using constants KPZDC and KPZDT. (Group H, Record 4, CONST(55), CONST(56))

Carbonaceous BOD Decomposition, day^{-1}-- The user may specify the rate constant and temperature coefficient for CBOD decomposition in benthic segments using constants KDSC and KDST

(Group H Record 4, CONST(73), CONST(74))

Organic Nitrogen Decomposition, day^{-1}-- The user may specify the rate constant and temperature coefficient for organic nitrogen decomposition in benthic segments using constants KONDC and KONDT (Group H, Record 4, CONST(93), CONST(94))

Organic Phosphorus Decomposition, day^{-1}-- The user may specify the rate constant and temperature coefficient for organic phosphorus decomposition in benthic segments using constants KOPDC and KOPDT (Group H, Record 4, CONST(102), CONST(103))

Data Group Descriptions

Input datasets to simulate eutrophication in a lake are given with the model software A comprehensive listing of the WASP5 data groups, records, and variables is given in Part B of this report

CHAPTER 6

SIMPLE TOXICANTS

6 1 MODEL DESCRIPTION

Introduction

Some organic and inorganic chemicals can cause toxicity to aquatic organisms, or bioconcentrate through the food chain Humans may be affected by ingesting contaminated water or fish Criteria for protecting human health and indiginous aquatic communities have been promulgated for specific chemicals and for general toxicity

The simulation of toxicants has become common only in the past decade Near-field mixing zone models simulate the dilution and dispersal of waste plumes along with associated toxicants Far-field models, such as WASP5, simulate the transport and ultimate fate of chemicals throughout a water body At a minimum these models simulate the water column and a bed layer, and include both chemical degradation and sorption to solids The simpler models use first-order decay constants and equilibrium partition coefficients More complex models may employ second-order decay mechanisms and either nonlinear sorption isotherms or first-order sorption and desorption rate constants

Several physical-chemical processes can affect the transport and fate of toxic chemicals in the aquatic environment Some chemicals undergo a complex set of reactions, while others behave in a more simplified manner WASP5 allows the simulation of a variety of processes that may affect toxic chemicals The model is designed to provide a broad framework applicable to many environmental problems and to allow the user to match the model complexity with the requirements of the problem

Although the potential amount and variety of data used by WASP5 is large data requirements for any particular simulation can be quite small For example it is possible to simulate a chemical using no reactions, or using only sorption and one or two transformation reactions that significantly affect a particular chemical Indeed for empirical studies, all chemical constants time functions, and environmental parameters can be ignored and a simple user-specified transformation rate constant used Thus, WASP5 can be used as a first-order water pollutant model to conduct simulations of dye tracers, salinity intrusion or coliform die-off

Overview of Simple WASP5 Toxicants

Simple toxicants and associated solids are simulated using the TOXI5 program TOXI5 simulates the transport and transformation of one to three chemicals and one to three types of particulate material (solids classes, Table 6 1) The three chemicals may be independent or they may be linked with reaction yields such as a parent compound-daughter product sequence The simulation of solids is described in Chapter 3 The simulation of simple toxicants is described below The simulation of more complex organic chemicals is described in Chapter 7

Table 6 1 WASP5 State Variables for Toxicants

SYSTEM	VARIABLE
1	CHEMICAL 1
2	SOLIDS 1
3	SOLIDS 2
4	SOLIDS 3
5	CHEMICAL 2
6	CHEMICAL 3

In an aquatic environment toxic chemicals may be transferred between phases and may be degraded by any of a number of chemical and biological processes Simplified transfer processes defined in the model include sorption and volatilization Transformation processes include biodegradation hydrolysis photolysis, and oxidation Sorption is treated as an equilibrium reaction The simplified transformation processes are described by first-order rate equations

WASP5 uses a mass balance equation to calculate sediment and chemical mass and concentrations for every segment in a specialized network that may include surface water, underlying water, surface bed, and underlying bed In a simulation, sediment is advected and dispersed among water segments, settled to and eroded from benthic segments, and moved between benthic segments through net sedimentation, erosion or bed load as detailed in Chapter 3

Simulated chemicals undergo several physical or chemical reactions as specified by the user in the input dataset Chemicals are advected and dispersed among water segments and exchanged with surficial benthic segments by dispersive mixing Sorbed chemicals settle through water column segments and deposit to or erode from surficial benthic segments Within the bed, dissolved chemicals migrate downward or upward through percolation and pore water diffusion Sorbed chemicals migrate downward or upward through net sedimentation or erosion Rate constants and equilibrium coefficients must be estimated from

Table 6 2 Concentration Related Symbols Used in Mathematical Equations

Symbol	Definition	Units
C_{ij}	Concentration of total chemical i in segment j	mg_c/L
$C_{w\,j}$	Concentration of dissolved chemical i in segment j	mg_c/L
C_{wij}	Concentration of dissolved chemical i in water in segment j $C_{wij} = C_{wij}/n_j$	mg_c/L_w
C_{sij}	Concentration of sorbed chemical i on sediment type s" in segment j	mg_c/L
$C_{s\,j}$	Concentration of sorbed chemical i on sediment type s" in segment j $C_{sij} = C_{sij}/M_{sij}$	mg_c/kg_s
m_{sj}	Concentration of sediment type s" in segment j	mg_s/L
M_{sj}	Concentration of sediment type "s in segment j $M_j = m_j \cdot 10^{6}$	kg_s/L
M_s	Concentration of sediment type s" in water in segment j	kg_s/L_w
n_j	Porosity or volume water per volume segment j	L_w/L
K_{ps}	Partition coefficient of chemical i on sediment type "s in segment j	L_w/kg_s
f_D	Fraction of chemical i in segment j in dissolved phase	-
f_s	Fraction of chemical i in segment j in solid phase 's"	-

field or literature data in simplified toxic chemical studies Their calculation from laboratory and field data is described in Chapter 7

Some limitations should be kept in mind when applying TOXI5 First, chemical concentrations should be near trace levels, i e below half the solubility or 10^{5} molar At higher concentrations the assumptions of linear partitioning and transformation begin to break down Chemical density may become important, particularly near the source, such as in a spill Large concentrations can affect key environmental characteristics, such as pH or bacterial populations, thus altering transformation rates

In TOXI5, it is convenient to define concentration related symbols as in Table 6 2 Please note that in the general development of the equations below subscripts i" and "j" are sometimese omitted for convenience

Simple Transformation Kinetics

TOXI5 allows the user to specify simple first-order reaction rates for the transformation reactions of each of the chemicals simulated First order rates may be applied to the total chemical and varied by segment Alternatively, constant first order rates may be specified for particular processes, including biodegradation, hydrolysis, photolysis, volatilization, and oxidation These constant rates may be used exclusively or in combination with model computed rates as described in Chapter 7 For example, the user may specify a first-order rate for biodegradation and have TOXI5 compute a loss rate for volatilization

Option 1 Total Lumped First Order Decay

The simplest rate expression allowed by TOXI5 is lumped first-order decay This option allows the user to specify spatially-variable first order decay rate constants (day ^{1}) for each of the chemicals simulated Because these are lumped decay reactions, chemical transformations to daughter products are not simulated

$$\frac{\partial C_{ij}}{\partial t}\bigg|_{reaction} = K_{ij}\ C_{ij} \tag{6 1}$$

where

K_{ij} = lumped first order decay constants (day ^{1}) for chemical i in segment j

The lumped decay rate constant is a model parameter that may be varied between model segments If a lumped decay rate constant is specified, the chemical will react at that rate regardless of other model input

Option 2 Individual First Order Transformation

This option allows the user to input a global first-order reaction rate constant separately for each of the following processes volatilization, water column biodegradation, benthic biodegradation, alkaline hydrolysis, neutral hydrolysis, acid hydrolysis, oxidation, photolysis, and an extra reaction The total reaction is then based on the sum of each of the individual reactions as given by

$$\frac{\partial C_{ij}}{\partial t}\bigg|_{reaction} = \sum_{k=1}^{N} K_{ki}\, C_{ij} \qquad 6\ 2$$

where

K_{ki} = first order transformation constants for reaction k of chemical i, day^{-1}

The user may input half-lives rather than first-order decay rate constants If half-lives are provided for the transformation reactions, they will be converted internally to first order rate constants and used as above

$$K_{ki} = 0\ 693 / T_{Hki} \qquad 6\ 3$$

where

T_{Hki} = half-life of reaction k for chemical i days

Equilibrium Sorption

Sorption is the bonding of dissolved chemicals onto solid phases, such as benthic and suspended sediment, biological material, and sometime dissolved or colloidal organic material Sorption can be important in controlling both the environmental fate and the toxicity of chemicals Sorption may cause the chemical to accumulate in bed sediment or bioconcentrate in fish Sorption may retard such reactions as volatilization and base hydrolysis, or enhance other reactions including photolysis and acid-catalyzed hydrolysis

Sorption reactions are usually fast relative to other environmental processes, and equilibrium may be assumed. For environmentally relevant concentrations (less than 10^{-5} M or one-half water solubility), equilibrium sorption is linear with dissolved chemical concentration (Karickhoff, 1984) or

$$C_s' = K_{ps} \; C_w' \qquad (6.4)$$

At equilibrium, then, the distribution among the phases is controlled by the partition coefficients K_{ps}. As developed in Chapter 7, the total mass of chemical in each phase is controlled by K_{ps} and the amount of solid phase present (ignoring here any DOC phase), so that

$$f_D = \frac{n}{n + \sum_s K_{ps} \; M_s} \qquad (6.5)$$

and

$$f_s = \frac{K_{ps} \; M_s}{n + \sum_s K_{ps} \; M_s} \qquad (6.5)$$

These fractions are determined in time and space throughout a simulation from the partition coefficients, internally calculated porosities and simulated sediment concentrations. Given the total concentration and the phase fractions of chemical i in segment j, the dissolved and sorbed concentrations are uniquely determined

$$C_{wij} = C_{ij} \; f_{Dij} \qquad (6.7)$$

$$C_{sij} = C_{ij} \; f_{sij} \qquad (6.8)$$

In addition to the assumption of instantaneous equilibrium implicit in the use of these equations is the assumption of reversibility. Laboratory data for very hydrophobic chemicals suggest, however, that a hysteresis exists with desorption being a much slower process than adsorption. Karickhoff suggests that this effect may be the result of intraparticle kinetics in which the chemical is slowly incorporated into components of the sorbant. This phenomenon is not well understood and no quantitative modeling framework is available to characterize it.

Values for the partition coefficients can be obtained from laboratory experiments or field data. TOXI5 allows the input of either a single constant partition coefficient, or a set of spatially-variable partition coefficients. These options are described under "Model Implementation" below. The calculation of partition coefficients for organic chemicals is described in Chapter 7.

Transformations and Daughter Products

The three chemicals that may be simulated by TOXI5 may be independent, or they may be linked with reaction yields, such as a parent compound-daughter product sequence. Linked transformations may be implemented by simulating two or three chemicals and by specifying appropriate yield coefficients for each process.

$$S_{kc1} = \sum_{c} \sum_{k} K_{kc}\, C_c\, Y_{kc1}\,, \qquad c = 2,3 \tag{6.9}$$

$$S_{kc2} = \sum_{c} \sum_{k} K_{kc}\, C_c\, Y_{kc2}\,, \qquad c = 1,3 \tag{6.10}$$

$$S_{kc3} = \sum_{c} \sum_{k} K_{kc}\, C_c\, Y_{kc3}\,, \qquad c = 1,2 \tag{6.11}$$

where

S_{kci} = production of chemical "i" from chemical c undergoing reaction k, mg/L-day

K_{kc} = effective rate coefficient for chemical "c reaction k," day^{-1}

Y_{kci} = yield coefficients for production of chemical i" from chemical c' undergoing reaction k," mg_i/mg_c

Figure 6.1 illustrates some of the linked reactions that can be simulated by specifying appropriate yield coefficients.

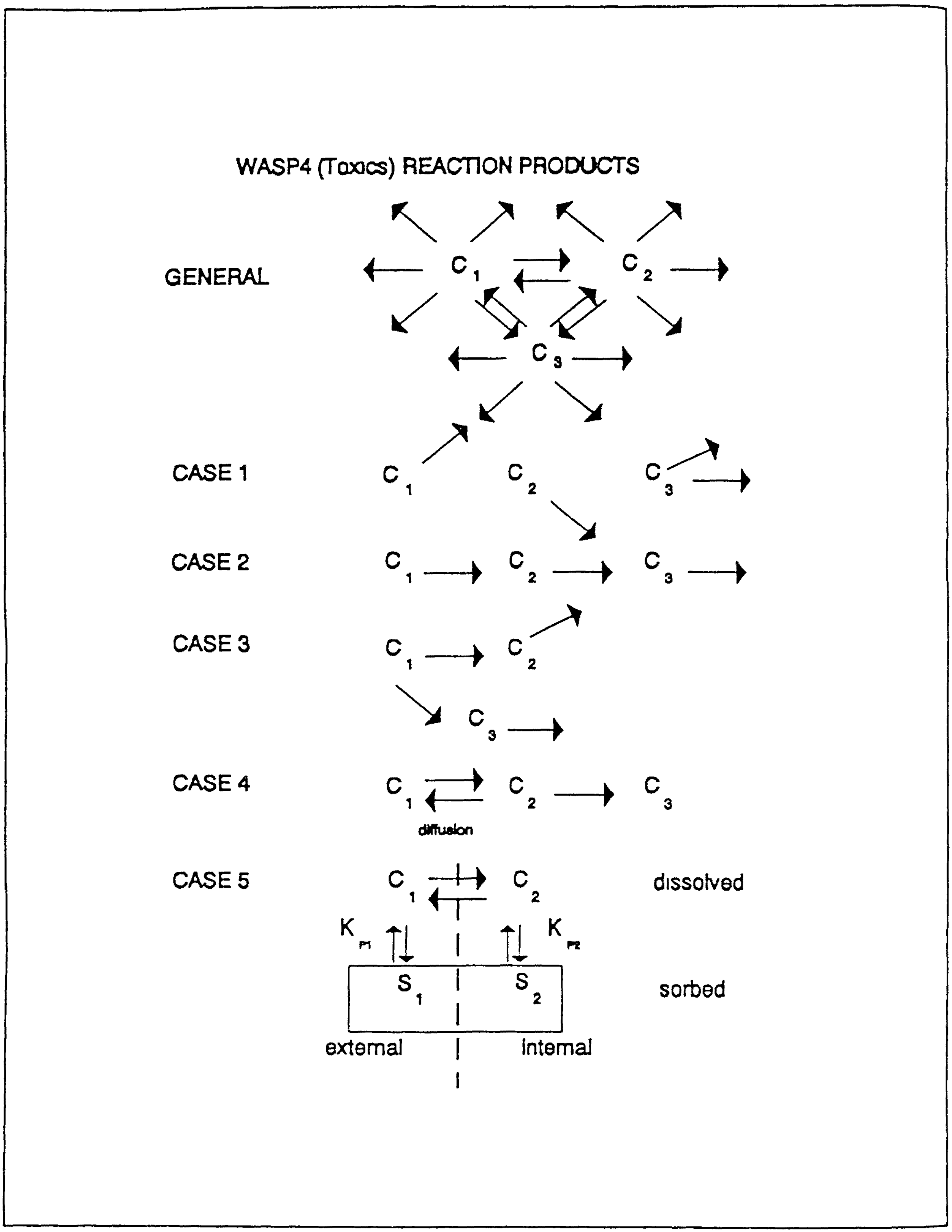


Figure 6 1 Potential Reaction Products in WASP5

6 2 MODEL IMPLEMENTATION

Introduction

To simulate simple toxicants with WASP5 use the preprocessor to create a TOXI5 input file The model input dataset and the input parameters will be similar to those for the conservative tracer model as described in Chapter 2 To those basic parameters, the user will add benthic segments, solids transport rates, and transformation parameters During the simulation, solids and toxicants will be transported both by the water column advection and dispersion rates and by these solids transport rates

In WASP5, solids transport rates in the water column and the bed are input via up to three solids transport fields, as described in Chapter 3 The transport of the particulate fraction of toxicants follows the solids flows The user must specify the dissolved fraction (i e 0 0) and the solids transport field for each simulated solid under initial conditions To simulate total solids solids 1 must be used

Model Input Parameters

This section summarizes the input parameters that must be specified in order to solve the simple toxicant equations in TOXI5 The user is referred to Chapter 3 for a summary of input parameters for the sediment balance equations Input parameters are prepared for WASP5 in four major sections of the preprocessor -- environment, transport, boundaries, and transformation Basic model parameters are described in Chapter 2 and will not be repeated here

Environment Parameters

These parameters define the basic model identity including the segmentation and control the simulation

Systems-- To simulate a toxicant, select 'simulate' for chemical 1 and bypass for chemical 2 and chemical 3 To simulate total solids along with the toxicant select 'simulate for solids 1 and "bypass" for solids 2 and solids 3 To simulate two or more toxicants or solids, select "simulate for the appropriate variable (Group A, Record 4, NOSYS, Record 9, SYSBY)

Bed Volume Option-- The user must determine whether bed volumes are to be held constant or allowed to vary Volumes may be held constant by specifying 0, in which case sediment concentrations and porosities in the bed segments will vary Alternatively, sediment concentrations and porosities may be held constant by specifying 1 in which case surficial bed segment volumes will vary (Group C Record 1, IBEDV)

Bed Time Step-- While mass transport calculations are repeated every model time step, certain benthic calculations are repeated only at this benthic time step, in days If the constant bed volume option is chosen, sediment concentrations are updated every model time step, but porosities are recalculated every benthic time step If the variable bed volume is chosen, upper benthic segment volumes are updated every time step, with compaction occurring every benthic time step (Group C, Record 1, TDINTS)

Transport Parameters

Number of Flow Fields-- Under advection, the user has a choice of up to six flow fields To simulate surface water toxicant and solids transport, select water column flow When simulating total solids the user should also select solids 1 flow To simulate three sediment types, the user should select solids 1 flow solids 2 flow, and solids 3 flow (Group D Record 1, NFIELD)

Water Column Flows, m^3/sec-- Time variable water column flows can be specified as detailed in Chapter 2 (Group D Record 6, QT, TQ, Record 4, BQ, JQ, IQ)

Sediment Transport Velocities, m/sec-- Time variable settling, deposition scour, and sedimentation velocities can be specified for each type of solid If the units conversion factor is set to 1 157e-5, then these velocities are input in units of m/day These velocities are multiplied internally by cross-sectional areas and treated as flows that carry solids and sorbed chemical between segments Settling velocities are important components of suspended sediment transport in the water column Scour and deposition velocities determine the transfer of solids and sorbed chemical between the water column and the sediment bed Sedimentation velocities represent the rate at which the bed is rising in response to net deposition (Group D, Record 6, QT, TQ)

Cross-Sectional Areas, m^2-- The interfacial surface area must be specified for adjoining segments where sediment transport occurs These surface areas are multiplied internally by sediment transport velocities to obtain sediment transport flows (Group D, Record 4 BQ, JQ IQ)

Number of Exchange Fields-- Under dispersion the user has a choice of up to two exchange fields To simulate surface water toxicant and solids dispersion, select water column dispersion To simulate exchange of dissolved toxicants with the bed the user should also select pore water diffusion (Group B Record

1, NRFLD)

Water Column Dispersion, m^3/sec-- Time variable water column dispersion can be specified, as detailed in Chapter 2 (Group B, Record 6, RT, TR, Record 4, A, EL)

Pore Water Diffusion Coefficients, m^2/sec-- Time variable pore water diffusion coefficients can be specified for dissolved toxicant exchange within the bed or between the bed and the water column If the units conversion factor is set to 1 157e-5, then these coefficients are input in units of m^2/day Diffusion coefficients are multiplied internally by cross-sectional areas divided by characteristic mixing lengths, and are treated as flows that carry dissolved toxicants between benthic segments and the water column (Group B, Record 6, RT, TR)

Cross-Sectional Areas, m^2-- The interfacial surface area must be specified for adjoining segments where pore water diffusion occurs These surface areas are multiplied internally by diffusion coefficients and divided by characteristic mixing lengths to obtain pore water exchange flows (Group B, Record 4 A)

Characteristic Mixing Lengths, m-- The characteristic mixing length must be specified for adjoining segments where pore water diffusion occurs The value for a mixing length is typically equal to the average depth of the pore water segments involved in the exchange These mixing lengths are divided into the product of the diffusion coefficients and cross-sectional areas to obtain pore water exchange flows (Group B, Record 4, EL)

Boundary Parameters

This group of parameters includes boundary concentrations, waste loads, and initial conditions Boundary concentrations must be specified for any segment receiving flow inputs, outputs, or exchanges Initial conditions includes not only initial concentrations but also the density and solids transport field for each solid and the dissolved fraction in each segment

Boundary Concentrations, mg/L-- At each segment boundary time variable concentrations must be specified for each toxicant and for each solids type simulated A boundary segment is characterized by water exchanges from outside the network, including tributary inflows, downstream outflows and open water dispersive exchanges (Group E, Record 4, BCT)

Waste Loads, kg/day-- For each point source discharge time variable toxicant and solids loads can be specified These loads can represent municipal and industrial wastewater discharges, or urban and agricultural runoff (Group F 1, Record 4, WKT)

Solids Transport Field-- The transport field associated with total solids or each solids type must be specified under initial conditions (Group J, Record 1, IFIELD)

Solid Density, g/cm^3-- The average density of the total sediment, or the density of each solids type must be specified This information is used to compute the porosity of benthic segments Porosity is a function of sediment concentration and the density of each solids type (Group J, Record 1, DSED)

Initial Concentrations, mg/L-- Concentrations of toxicant and each solids type in each segment must be specified for the time at which the simulation begins If the variable benthic volume option is used, the benthic sediment concentrations specified here will remain constant for the entire simulation (Group J Record 2, C)

Dissolved Fraction-- The dissolved fraction of each solid in each segment should be set to 0 The dissolved fraction of toxicant will be controlled by the partition coefficient and solids concentrations (Group J, Record 2, DISSF)

Transformation Parameters

This group of parameters includes spatially variable parameters constants and kinetic time functions for the water quality constituents being simulated None are necessary for sediment transport

First-Order Degradation-- There are two options to input first-order toxicant degradation

Option 1 Total Lumped First Order Decay

The use of the simple lumped first-order decay rate requires the user to input a decay rate constant for the chemical for each model segment If a simple lumped first order rate is specified for a particular chemical, the chemical will decay at that rate regardless of other input For example if both a lumped decay rate and either a simple first order or second order transformation rate are specified the simple first or second order rates will only be used if the lumped rate is zero (Group G, Record 4, PARAM(ISEG 16), PARAM(ISEG, 17) PARAM(ISEG 18)

Option 2 Individual First Order Transformation

The use of the simple first-order transformation rate requires the user to input a global rate constant (day^{-1}) or half-life (day) for each particular processes simulated If a simple first-order transformation rate is specified, it will take priority over other input for that particular processes For example if both a first order and a second order transformation

Table 6 3   TOXI5 Rate Coefficients for Simple Reactions

Constant	C_1	C_2	C_3	REACTION
KV, day ^{1}	140	740	1340	Volatilization
THV, day	145?	745?	1345?	
KBW, day ^{1}	141	741	1341	Water Column Biodegradation
THBW, day	143	743	1343	
KBS, day ^{1}	142	742	1342	Benthic Biodegradation
THBS, day	144	744	1344	
KHOH, day ^{1}	181	781	1381	Alkaline Hydrolysis
THHOH, day	252	852	1452	
KHN day ^{1}	182	782	1382	Neutral Hydrolysis
THHN, day	253	853	1453	
KHH, day ^{1}	183	783	1383	Acid Hydrolysis
THHH, day	254	854	1454	
KO day ^{1}	256	856	1456	Oxidation
THO, day	257	857	1457	
KF, day ^{1}	287	887	1482	Photolysis
THF, day	289	889	1489	
KE, day ^{1}	571	1171	1771	Extra Reaction
THE day	572	1172	1772	

rate constant is specified the second order rate will only be used if the first-order rate constant is zero First-order transformation rate constant numbers are given in Table 6 3 (Group H Record 4 CONST(i))

Partition Coefficients-- TOXI5 allows the input of either a single constant partition coefficient, or a set of spatially-variable partition coefficients

Option 1 Constant Partition Coefficient

This option allows the user to directly input constant partition coefficients that apply over the entire model network These partition coefficients are input using the set of constants PIXC, in units of L_w/kg_s (not in log units) If only one chemical and one solids type is being simulated, then the partition coefficient can be input by specifying a value for Constant 111 -- PIXC(1,1). All other partitioning information should be omitted (i.e. - LKOW, LKOC, and FOC).

If three chemicals are being simulated, the user may specify values for their partition coefficients to solids 1 using three separate PIXC values -- Constants 111, 711, and 1311, respectively.

Coefficients PIXC

	C_1	C_2	C_3
Solids 1	111	711	1311
Solids 2	116	716	1316
Solids 3	121	721	1321

If multiple solids types are being simulated, then separate partition coefficients may be input for each of the three solids types. The constant partition coefficients for chemical 1 to solids type 2 and 3 can be input by specifying appropriate PIXC values for Constants 116 and 121, respectively.

Constant numbers for partitioning of chemical i to solid j are summarized in Table 6.4.

Option 2. Spatially-Variable Partition Coefficients

This option allows the user to directly input spatially-variable partition coefficients for chemical 1. These partition coefficients are input using the parameter FOC, in units of L_w/kg_s (not in log units). If only one chemical and one solids type is being simulated then the partition coefficients can be input by specifying segment-variable values for Parameter 7 -- FOC(ISEG,1). Constant 101, LKOC, should be given a small nonzero value, such as 1.0e-20.

If multiple solids types are being simulated then separate sets of partition coefficients may be input for each of the three solids types. The constant partition coefficients for chemical 1 to solids type 2 and 3 can be input by specifying segment-variable values for FOC(ISEG,2) and FOC(ISEG,3) -- Parameters 8 and 9, respectively.

Reaction Yields-- The input yield constants that may be specified are $YHOH_{ci}$, YHN_{ci}, YHH_{ci}, YBW_{ci}, YBS_{ci}, YF_c, YOX_{ci}, and YE, where c is the chemical reactant (1, 2, or 3) and i is the chemical product (1, 2, or 3) in units of mg_c/mg_i. Yield coefficients may be provided for all possible combinations of chemicals and for the reactions, as listed in Table 6.5.

Table 6 5 TOXI5 Yield Constants for Chemical Reactions

FROM	to C_1	to C	to C_3	REACTION
C_1		176	177	Water Column Biodegradation YBW_{ci}
C_2	776		777	
C_3	1376	1377		
C_1		178	179	Benthic Biodegradation YBS_{ci}
C_2	778		779	
C_3	1378	1379		
C_1		246	247	Alkaline Hydrolysis $YHOH_{ci}$
C_2	846		847	
C_3	1446	1447		
C_1		248	249	Neutral Hydrolysis YHN_{ci}
C_2	848		849	
C_3	1448	1449		
C_1		250	251	Acid Hydrolysis YHH_{ci}
C_2	850		851	
C_3	1450	1451		
C_1		281	282	Oxidation YOX_{ci}
C_2	881		882	
C_3	1481	1482		
C_1		566	567	Photolysis YF_c
C_2	1166		1167	
C_3	1766	1767		
C_1		596	597	Extra Reaction YE_{ci}
C_2	1196		1197	
C_3	1796	1797		

CHAPTER 7

ORGANIC CHEMICALS

7 1 MODEL DESCRIPTION

Introduction

In modern technological societies, synthetic organic chemicals have been manufactured, used, and disposed of in large quantities The large number and variety of organic compounds include such major classes as pesticides, polychlorinated biphenyls, halogenated aliphatic hydrocarbons, halogenated ethers monocyclic aromatics, phthalate esters, polycyclic aromatic hydrocarbons, and nitrosamines Organic chemicals can enter the aquatic environment by various pathways, including point source waste discharges and nonpoint source runoff Some of these organic chemicals can cause toxicity to aquatic organisms, or bioconcentrate through the food chain Humans may be affected by ingesting contaminated water or fish Criteria for protecting human health and indiginous aquatic communities have been promulgated for some organic chemicals

Several environmental processes can affect the transport and fate of organic chemicals in the aquatic environment The most important include physical processes such as hydrophobic sorption, volatilization, and sedimentation, chemical processes such as ionization, precipitation, dissolution hydrolysis photolysis, oxidation and reduction, and biological processes such as biodegradation and bioconcentration WASP5 explicitly handles most of these, excluding only reduction and precipitation-dissolution If the kinetics of these reactions are described by the user, they also can be included as an extra reaction

WASP5 allows the simulation of a variety of processes that may affect toxic chemicals However, WASP5 makes relatively few assumptions concerning the particular processes affecting the transport, transformations and kinetic reactions The model is designed to provide a broad framework applicable to many environmental problems and to allow the user to match the model complexity with the requirements of the problem

Although the potential amount and variety of data used by WASP5 is large data requirements for any particular simulation can be quite small Most often, organic chemical simulations use only sorption and one or two transformation processes that significantly affect a particular chemical What is gained by the second-order process functions and resulting input data burden is the ability to extrapolate more confidently to future conditions The user must determine the optimum amount of empirical calibration and process specification for each application

Overview of WASP5 Organic Chemicals

Organic chemicals and associated solids are simulated using the TOXI5 program TOXI5 simulates the transport and transformation of one to three chemicals and one to three types of particulate material (solids classes, Table 7 1) The three chemicals may be independent or they may be linked with reaction yields, such as a parent compound-daughter product sequence The simulation of solids is described in Chapter 3 The simulation of organic chemicals is described below Organic chemical process routines are closely derived from the Exposure Analysis Modeling System EXAMS (Burns, et al , 1982, Burns, 1986)

Table 7 1 TOXI5 State Variables for Toxicants

SYSTEM	VARIABLE
1	CHEMICAL 1
2	SOLIDS 1
3	SOLIDS 2
4	SOLIDS 3
5	CHEMICAL 2
6	CHEMICAL 3

Each organic chemical may exist as a neutral compound and up to four ionic species The neutral and ionic species can exist in five phases dissolved, sorbed to dissolved organic carbon (DOC), and sorbed to each of the up to three types of solids (Figure 7 1) Local equilibrium is assumed so that the distribution of the chemical between each of the species and phases is defined by distribution or partition coefficients In this fashion, the concentration of any specie in any phase can be calculated from the total chemical concentration Therefore only a single state variable (WASP system) representing total concentration is required for each chemical The model, then, is composed of up to six systems -- three chemicals and three solids -- for which the general WASP5 mass balance equation is solved

There are often other factors that may influence the transport and transformations of the chemicals simulated For example, water temperature affects reaction kinetics, sorption may also occur onto dissolved organic carbon, and pH can affect ionization and hydrolysis reactions These concentrations or properties are included in TOXI5 through the use of model parameters and time functions They are specified to the model (described) rather than simulated They may be varied over space

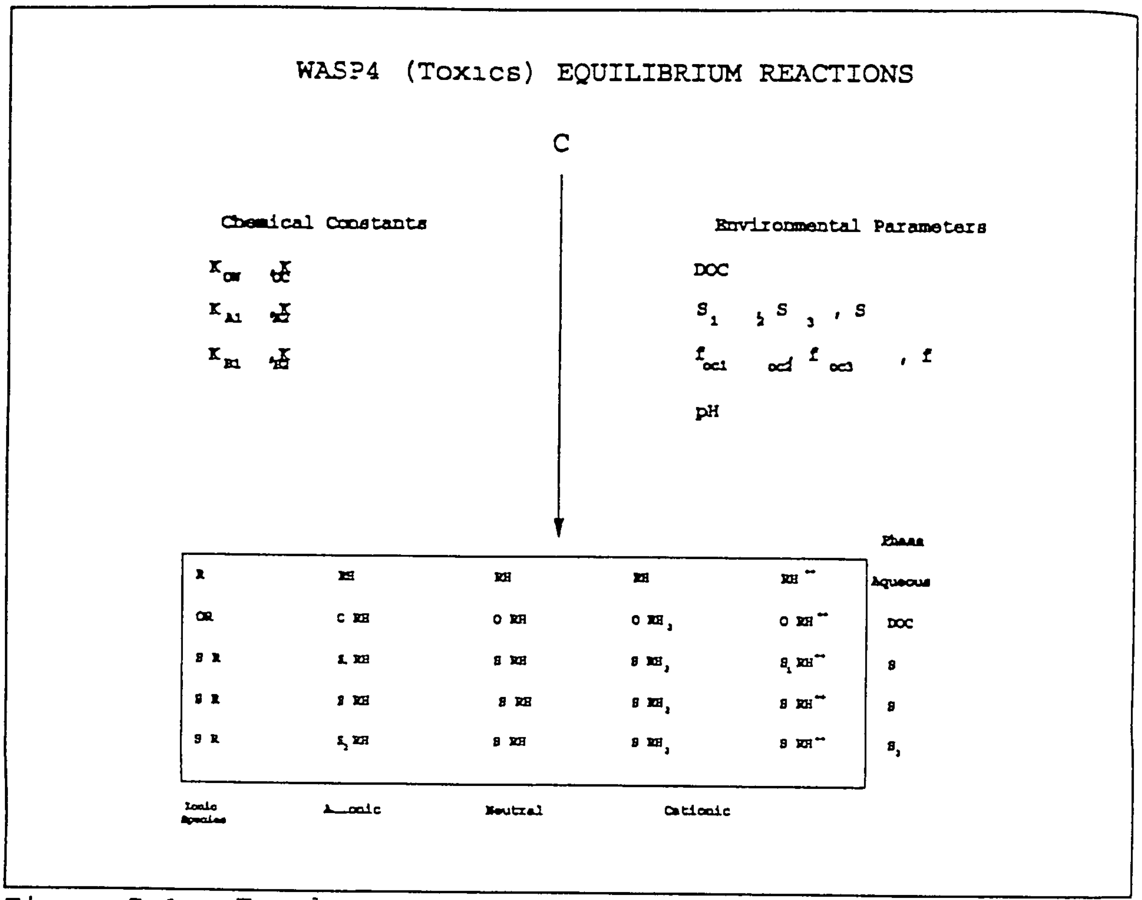


Figure 7 1 Equilibrium speciation

(e g between model segments) and/or over time Examples of the concentrations or properties that are described to the model are provided in Table 7 2

TOXI5 Reactions and Transformations

In an aquatic environment an organic chemical may be transferred between phases and may be degraded by any of a number of chemical and biological processes Ionization may speciate the chemical into multiple forms Transfer processes defined in the model include sorption and volatilization Defined transformation processes include biodegradation, hydrolysis, photolysis and chemical oxidation Sorption and ionization are treated as equilibrium reactions All other processes are described by rate equations Rate equations may be quantified by first-order constants or by second-order chemical specific constants and environment-specific parameters that may vary in space and time

Table 7 2 Examples of TOXI5 Parameters and Time Functions

Parameter or Time Function	Units	Time Variable	Affected Kinetic Processes
Water Temperature	°C	Y	All
Dissolved Organic Carbon	mg/L	N	Sorption, Photolysis
Fraction Organic Carbon	none	N	Sorption
pH	-	Y	Hydrolysis
Oxidant Concentration	moles/L	N	Oxidation
Bacterial Concentration	variable	Y	Biodegradation
Extra Property	variable	N	Extra 2nd Order Reaction
Wind Velocity	m/sec	Y	Volatilization
Air Temperature	°C	Y	Volatilization
Chlorophyll *a* Concentration	mg/L	Y	Photolysis
Normalized Light Intensity	None	Y	Photolysis (Option 2 Only)

WASP5 uses a mass balance equation to calculate sediment and chemical mass and concentrations for every segment in a specialized network that may include surface water, underlying water, surface bed, and underlying bed In a simulation sediment is advected and dispersed among water segments, settles to and erodes from benthic segments and moves between benthic segments through net sedimentation, erosion, or bed load Chapter 3 details the TOXI5 sediment transport processes

In a simulation the chemical can undergo several physical or chemical transformations It is convenient to group these into fast and slow reactions Fast reactions have characteristi reaction times that are much faster than, or on the same order o the model time step and are handled with the assumption of local equilibrium Slow reactions have characteristic reaction times much longer than the model time step These are handled with the assumption of local first order kinetics using a lumped rate constant specified by the user, or calculated internally, based on summation of several process rates, some of which are second-order Thus, the effective first order decay rate can vary with time, and space, and is recalculated as often as necessary throughout a simulation

The chemical is advected and dispersed among water segments and exchanged with surficial benthic segments by dispersive mixing Sorbed chemical settles through water column segments and deposits to or erodes from surficial benthic segments Within the bed, dissolved chemical migrates downward or upward through percolation and pore water diffusion Sorbed chemical migrates downward or upward through net sedimentation or erosion Both rate constants and equilibrium coefficients must be estimated in most toxic chemical studies Although these can be calculated internally from chemical properties and local environmental characteristics, site-specific calibration or testing is desirable

Some limitations should be kept in mind when applying TOXI5 First, chemical concentrations should be near trace levels, i e below half the solubility or 10^{5} molar At higher concentrations, the assumptions of linear partitioning and transformation begin to break down Chemical density may become important particularly near the source, such as in a spill Large concentrations can affect key environmental characteristics, such as pH or bacterial populations thus altering transformation rates TOXI5 does not include such feedback phenomena

7 2 MODEL IMPLEMENTATION

Introduction

To simulate organic chemicals with WASP5, use the preprocessor or text editor to create a TOXI5 input file The model input dataset and the input parameters will be similar to those for the conservative tracer model as described in Chapter 2 To those basic parameters, the user will add benthic segments solids transport rates and transformation parameters During the simulation, solids and organic chemicals will be transported both by the water column advection and dispersion rates and by these solids transport rates

In WASP5, solids transport rates in the water column and the bed are input via up to three solids transport fields as described in Chapter 3 The transport of the particulate fraction of organic chemicals follows the solids flows The user must specify the dissolved fraction (i e 0 0) and the solids transport field for each simulated solid under initial conditions To simulate total solids, solids 1 must be used

Model Input Parameters

Input parameters are prepared for WASP5 in four major sections of the preprocessor -- environment, transport, boundaries, and transformation The organic chemical input parameters comprising the first three sections are identical to those in the simple toxicant model The user is referred to Section 6 2 for a summary of these input parameters This section, and the rest of this chapter, describes the organic chemical reaction parameters

Transformation Parameters

This group of parameters includes spatially variable parameters, constants, and kinetic time functions for the water quality constituents being simulated The organic chemical reactions and model input parameters are described in individual sections below Because water temperature can affect every chemical reaction, it is described here

Water Temperature, [illegible]-- Water temperature can vary in space and time, affecting the rates of all chemical reactions Time and segment variable water temperatures can be specified using the parameters TEMP and TMPFN and the time functions TEMPN(1-4) If temperatures are to remain constant in time, then the user should enter segment temperatures using the parameter TEMP TMPFN and TEMPN(1-4) should be omitted

If the user wants to enter time-variable temperatures then values for the parameter TEMP should be set to 1 0 The parameter TMPFN indicates which temperature function will be used by the model for each segment Values of 1 0 2 0 3 0 or 4 0 will call time functions TEMPN(1) TEMPN(2), TEMPN(3) and TEMPN(4), respectively Water temperatures should then be entered via these time functions as a series of temperature versus time values The product of TEMP and the selected TEMPN function will give the segment and time specific water temperatures used by TOXI5

TEMP and TMPFN are identified in TOXI5 as parameters 3 and 2 respectively TEMPN(1-4) are identified in TOXI5 as time functions 1-4 (Group G, Record 4, PARAM(I,3) PARAM(I,2), Group I, Record 2 VALT(1-4 K))

Table 7 3 Concentration Related Symbols Used in Mathematical Equations

Symbol	Definition	Units
C_{ij}	Concentration of total chemical i in segment j	mg_c/L
C_{wij}	Concentration of dissolved chemical i in segment j	mg_c/L
C_{wij}	Concentration of dissolved chemical i in water in segment j, C_{wij}/n_j	mg_c/L_w
C_{sij}	Concentration of sorbed chemical i on sediment type "s" in segment j	mg_c/L
C_{sij}	Concentration of sorbed chemical i on sediment type s" in segment j, C_{sij}/M_{sij}	mg_c/kg_s
C_{Bj}	Concentration of DOC-sorbed chemical i in segment j	mg_c/L
C_{Bj}	Concentration of DOC-sorbed chemical i in segment j, C_{Bj}/B_j	mg_c/kg_B
m_{sj}	Concentration of sediment type "s in segment j	mg_s/L
M_{sj}	Concentration of sediment type "s" in segment j $m_s \cdot 10^{6}$	kg_s/L
M_{sj}	Concentration of sediment type "s" in water in segment j, M_{sj}/n	kg_s/L_w
B	Concentration of DOC in segment j	kg_B/L
B_j	Concentration of DOC in water in segment j, B_j/n	kg_B/L_w
n_j	Porosity or volume water per volume segment j	L /L
K_{psj}	Partition coefficient of chemical i on sediment type 's in segment j	L /kg_s
K_{Bj}	Partition coefficient of chemical i on DOC in segment j	L /kg_B
f_{Dj}	Fraction of chemical i in segment j in dissolved phase	-
f_{Bij}	Fraction of chemical i in segment j in DOC-sorbed phase	-
f_{sj}	Fraction of chemical i in segment j in solid phase s"	-

Notation

In TOXI5, it is convenient to define concentration related symbols as in Table 7 3 Please note that in the general development of the equations in the sections below, subscripts "i" and "j are sometimes omitted for convenience

7 3 IONIZATION

Introduction

Ionization is the dissociation of a chemical into multiple charged species In an aquatic environment some chemicals may occur only in their neutral form while others may react with water molecules to form positively (cationic) or negatively (anionic) charged ions These reactions are rapid and are generally assumed to be at (local) equilibrium At equilibrium the distribution of chemicals between the neutral and the ionized species is controlled by the pH and temperature of the water and the ionization constants

Ionization can be important because of the different toxicological and chemical properties of the neutral and ionized species For example, in some cases only the neutral form of the chemical may react or be transported through biotic membranes resulting in toxicity As a result, it is often necessary to compute the distribution of chemicals among ionic forms as well as to allow them to react or transform at different rates For example in TOXI5 different sorption and reaction constants (e g for hydrolysis, biodegradation, photolysis, etc) may be specified for each ionic form of the chemical

Overview of TOXI5 Ionization Reactions

In TOXI5, each of the three possible chemicals being simulated may occur in up to five forms, including 1) the neutral molecule 2) singly charged cations 3) doubly charged cations 4) singly charged anions, and 5) doubly charged anions Each of the neutral or ionic species may also occur in the dissolved phase or sorbed to dissolved organic carbon (DOC) or the three solids types A total of 25 forms of each chemical may occur Each chemical form may have different reactivities as reflected by different degradation or transformation rates TOXI5 makes no direct assumptions as to the formation of the ionic species or their reactivity The formation is controlled by the user by specification of model input

A chemical being modeled by TOXI5 is presumed to exist as neutral molecules that may or may not react with water molecules to form singly and, possibly, doubly charged cations and anions To illustrate an organic acid (A) may react with water as described by

$$AH_2 + H_2O \rightleftharpoons AH_3^+ + OH^- \quad (7\ 7)$$

$$AH_3^+ + H_2O \rightleftharpoons AH_4^{++} + OH^- \quad (7\ 8)$$

$$AH_2 + H_20 \rightleftharpoons AH^- + H_3O^+ \quad (7\ 9)$$

$$AH^- + H_2O \rightleftharpoons A^{--} + H_3O^+ \quad (7\ 10)$$

so that the chemical may exist in from one to a maximum of five species simultaneously (A^- , AH , AH_2 AH_3^+, AH_4^{++}) The law of mass action can be used to describe local chemical equilibrium for each of these reactions

$$K_{b_1} = \frac{[AH_3^+]\,[OH^-]}{[AH_2]} \quad (7\ 11)$$

$$K_{b_2} = \frac{[AH_4^{++}]\,[OH^-]}{[AH_3^+]} \quad (7\ 12)$$

$$K_{a_1} = \frac{[AH^-]\,[H^+]}{[AH_2]} \quad (7\ 13)$$

$$K_{a_2} = \frac{[A^{--}]\,[H^+]}{[AH^-]} \quad (7\ 14)$$

where K is the equilibrium constant for the formation of the acid (K_{a1}), or anionic species or the base (K_{b1}) or cationic species

The total concentration of the particular chemical is the sum of the concentration of each of these forms as given by

$$C = AH_2 + AH_3^+ + AH_4^{++} + AH^- + A^{--} \qquad (7\ 15)$$

which may be combined with the law of mass action to form

$$C = AH_2 \left[\frac{K_{b1}}{[OH^-]} + \frac{K_{b1}K_{b2}}{[OH^-]^2} + \frac{K_{a1}}{[H^+]} + \frac{K_{a1}K_{a2}}{[H^+]^2} \right] \qquad (7\ 16)$$

By definition, $[H^+] = 10^{\ pH}$ and $[OH\ ] = 10^{14\ pH}$, the bracketed term in equation 7 10, denoted D, can be written

$$D = \left[\frac{K_{b1}}{10^{pH-14}} + \frac{K_{b1}K_{b2}}{(10^{pH-14})^2} + \frac{K_{a1}}{10^{-pH}} + \frac{K_{a1}K_{a2}}{(10^{-pH})^2} \right] \qquad (7\ 17)$$

Equations 7 10 and 7 11 may be combined with equations 7 5 - 7 8 and solved for the fraction of the total chemical f^k occurring in each of the chemical species k, given the total chemical concentration the pH, and the equilibrium constants

$$f^0 = \frac{1}{D} \qquad (7\ 18)$$

$$f^+ = \frac{K_{b1}/10^{pH-14}}{D} \qquad (7\ 19)$$

$$f^{++} = \frac{K_{b1}K_{b2}/(10^{pH-14})^2}{D} \qquad (7\ 20)$$

$$f^- = \frac{K_{a1}/10^{-pH}}{D} \qquad (7\ 21)$$

$$f^{--} = \frac{K_{a1}K_{a2}/(10^{-pH})^2}{D} \qquad (7\ 22)$$

The rates of chemical reactions may also vary with temperature so that the equilibrium constants are a function of temperature The functional dependence of these constants on temperature may be described by the Van't Hoff equation

$$\frac{d\ln K_i}{dT_K} = \frac{E_{ai}}{RT_K^2} \qquad (7\ 23)$$

or in its integrated form

$$\log K_i(T_K) = \log K_i(T_{Ri}) + \frac{E_{ai}}{2\ 303\ R}\left[\frac{T_K - T_{Ri}}{T_K T_{Ri}}\right] = -\,pK_{ai} + \frac{E_{ai}}{2\ 303\ R}\left[\frac{T_K - T_{Ri}}{T_k T_{Ri}}\right] \qquad (7\ 24)$$

where

K_i = equilibrium constant
A_i = frequency factor
E_{ai} = standard enthalpy change for reaction, kcal/mole
R = the universal gas constant, kcal/mole 袁
T = water temperature 袁
T_{Ri} = reference temperature at which input ionization reaction constant was observed 袁

Table 7 4 TOXI5 Ionization Data

Description	Notation	Common Range	S I Units
Negative log of hydrogen ion activity [H]	pH	5-9	-
Negative log of ionization constants for acid	pK_a	-	-
Negative log of ionization constants for base	pK	-	-
Enthalpy change for ionization reactions	E_{ai}	4-8	kcal/mole
Water temperature	T	4-30	蚓
Reference temperature	T_{Ri}	20-25	蚓

Implementation

The data required for the implementation of ionization in TOXI5 are summarized in Table 7 4 They include first identifying whether or not a particular ionic specie is to be included in the simulation and then, if a particular specie is selected, the information necessary to compute its formation For example, to compute a particular ionic specie, it is necessary to input the pK (negative log) of the equilibrium constant for the formation of the acid and/or base, and the activation energy used in the Van t Hoff Equation to adjust the equilibrium constant with temperature If the activation energy is not input, then no temperature correction will occur If no data are input for ionization, none will occur and the reactions and transformations will be applied to the total or dissolved form of the chemical as appropriate

In addition to the constants for the formation of the ionic species, the pH and temperature (if the rate is to be temperature corrected) are required The pH and temperature are model parameters, which are specified for each model segment They may be constant or time variable

If ionization is specified in input, separate transformation and reaction rates may be specified for each ionic specie For example, where necessary, different sorption biodegradation, hydrolysis, oxidation, and photolysis constants may be specified for each ionic specie, providing considerable flexibility in the model application

The transformation input parameters for ionization are summarized below Constant numbers are given in Table 7 5

Ionization Switches-- The user may choose to simulate ionic species by specifying values of 1 0 for constant SFLG

Ionization Constants-- For each ionic specie being simulated, the user should provide a value for the negative log of the frequency factor in the Van't Hoff equation using constant PKA If the activation energy is 0 then this is equivalent to the pK_a or pK_b

Reaction Enthalpy, kcal/mole-- To simulate temperature dependence for ionization the user can specify the standard enthalpy change of the dissociation reaction using constant EPKA Higher reaction enthalpies cause more temperature dependence

pH-- The user may specify segment and time variable bacterial concentrations using parameter 11, PH, and time funcions 10 and 11, PHNW and PHNS If pH is to remain constant in time, the user should enter segment mean values using parameter PH PHNW and PHNS should be omitted

The user may enter time-variable water column and benthic p-

Table 7 5 TOXI5 Constants for Ionization Reactions

IONIC SPECIE "i"	C_1	C_2	C_3	INPUT VARIABLE
+	85	685	1285	Species Flag, $SFLG_i$
++	86	686	1286	
-	87	687	1287	
--	88	688	1288	
+	91	691	1291	Negative Log of Ionization Constant, PKA_i
++	92	692	1292	
-	93	693	1293	
--	94	694	1294	
+	95	695	1295	Ionization Reaction Enthalpy, $EPKA_i$, kcal/mole
++	96	696	1296	
-	97	697	1297	
--	98	698	1298	
All	99	699	1299	Reference Temp TREFI 蚓

values via time functions PHNW and PHNS, respectively as a series of concentration versus time values Parameter PH will then represent the ratio of each segment pH to the time function values The product of PH and the PHNW or PHNS function gives the segment and time specific pH values used by TOXI5 (Group G Record 4, PARAM(I,11), Group I, Record 2 VALT(10,K), VALT(11,K))

7 4 EQUILIBRIUM SORPTION

Introduction

Sorption is the binding of dissolved chemicals onto solid phases, such as benthic and suspended sediment, biological material and sometime dissolved or colloidal organic material Sorption can be important in controlling both the environmental fate and the toxicity of chemicals Sorption may cause the chemical to accumulate in bed sediment or bioconcentrate in fish Sorption may retard such reactions as volatilization and base hydrolysis or enhance other reactions including photolysis and acid-catalyzed hydrolysis

Sorption reactions are usually fast relative to other environmental processes and equilibrium may be assumed. For environmentally relevant concentrations (less than 10^{-5} M or one-half water solubility), equilibrium sorption is linear with dissolved chemical concentration (Karickhoff, 1984) or

$$C_s = K_{ps} \quad C_w \qquad (7.25)$$

At equilibrium, then, the distribution among the phases is controlled by the partition coefficients K_{ps}. The total mass of chemical in each phase is controlled by K_{ps} and the amount of solid phase present (including any DOC phase).

In addition to the assumption of instantaneous equilibrium, implicit in the use of equation 7.19 is the assumption of reversibility. Laboratory data for very hydrophobic chemicals suggest, however, that a hysteresis exists, with desorption being a much slower process than adsorption. Karickhoff suggests that this effect may be the result of intraparticle kinetics in which the chemical is slowly incorporated into components of the sorbant. This phenomenon is not well understood and no quantitative modeling framework is available to characterize it.

Overview of TOXI5 Sorption Reactions

Dissolved chemical in water column and benthic segments interacts with sediment particles and dissolved organic carbon to form five phases-- dissolved, DOC-sorbed, and sediment-sorbed (three sediment types "s"). The reactions can be written with respect to unit volume of water:

$$M_s + C_w \leftrightarrow C_s/n \qquad (7.26)$$

$$B + C_w \leftrightarrow C_B/n \qquad (7.27)$$

where n is the porosity (volume of water divided by total volume),

The forward reaction is sorption and the backward reaction is desorption. These reactions are usually fast in comparison with the model time step, and can be considered in local equilibrium. The phase concentrations C_w, C_s, and C_B are governed by the equilibrium partition coefficients K_{ps0} and K_{pB} (L/kg).

$$K_{ps0} = \frac{C_s/n}{M_s \; C_w} = \frac{C_s}{C_w} \qquad (7\ 28)$$

$$K_{pB} = \frac{C_B/n}{B \; C_w} = \frac{C_B}{C_w} \qquad (7\ 29)$$

These equations give the linear form of the Freundlich isotherm, applicable when sorption sites on sediment and DOC are plentiful

$$C_s = K_{ps} \, C_w \qquad (7\ 30)$$

$$C_B = K_{pB} \, C_w \qquad (7\ 31)$$

The total chemical concentration is the sum of the five phase concentrations

$$C = C_w \, n + \sum_s C_s \, M_s + C_B \, B \qquad (7\ 32)$$

Substituting in equations 7 24 and 7 25 factoring and rearranging terms gives the dissolved fraction f_D

$$f_D = \frac{C_w \, n}{C} = \frac{n}{n + K_{pB} \; B + \sum_s K_{ps} \; M_s} \qquad (7\ 33)$$

Similarly the sediment-sorbed and DOC-sorbed fractions are

$$f_s = \frac{C_s \, M_s}{C} = \frac{K_{ps} \; M_s}{n + K_{pB} \; B + \sum_s K_{ps} \; M_s} \qquad (7\ 34)$$

$$f_B = \frac{C_B \, B}{C} = \frac{K_{pB} \; B}{n + K_{pB} \; B + \sum_s K_{ps} \; M_s} \qquad (7\ 35)$$

These fractions are determined in time and space throughout a simulation from the partition coefficients, internally calculated porosities, simulated sediment concentrations, and specified DOC concentrations. Given the total concentration and the five phase fractions, the dissolved, sorbed, and biosorbed concentrations are uniquely determined:

$$C_w = C \cdot f_D \qquad (7.36)$$

$$C_S = C \cdot f_S \qquad (7.37)$$

$$C_B = C \cdot f_B \qquad (7.38)$$

These five concentrations have units of mg/L and can be expressed as concentrations within each phase:

$$C_w = C_w/n \qquad (7.39)$$

$$C_S = C_S/M_S \qquad (7.40)$$

$$C_B = C_B/B \qquad (7.41)$$

These concentrations have units of mg/L_w, mg/kg_s, and mg/kg_B, respectively.

In some cases, such as near discharges, the user may have to alter input partition coefficients to describe the effect of incomplete sorption. As guidance, Karickhoff and Morris (1985) found that typical sorption reaction times are related to the partition coefficient:

$$k_d^{-1} = 0.03\ k_{ps} \qquad (7.42)$$

where k_d^{-1} is the desorption rate constant, hr^{-1}.

Thus, compounds with high, medium, and low K_{ow}'s of 10^5, 10^3, and 10 sorbing onto 2% organic sediment should have reaction times of a day, a half hour, and seconds. Given that time to equilibrium is roughly three times the reaction time, the three compounds should reach equilibrium within 3 days, 1 hour, and 30 minutes

Computation of Partition Coefficients

Values for the partition coefficients can be obtained from laboratory experiments For organic chemicals, lab studies have shown that the partition coefficient is related to the hydrophobicity of the chemical and the organic matter content of the sediment TOXI5 provides several optional methods for the description or computation of the partition coefficients These options are identified by the data input, as described below

Option 1 Measured Partition Coefficients

This option allows the user to directly input a partition coefficient Separate partition coefficients may be input for each of the three solids types The partition coefficient is input in units of L_w/kg_s (**not** in log units)

Option 2 Input of Organic Carbon Partition Coefficient

Normalization of the partition coefficient by the organic-carbon content of the sediment has been shown to yield a coefficient K_{oc} (the organic carbon partition coefficient) that is relatively independent of other sediment characteristics or geographic origin Many organic pollutants of current interest are non-polar, hydrophobic compounds whose partition coefficients correlate quite well with the organic fraction of the sediment Rao and Davidson (1980) and Karickhoff et al (1979) have developed empirical expressions relating equilibrium coefficients to laboratory measurements leading to fairly reliable means of estimating appropriate values The correlations used in TOXI5 are

$$K_{ps0} = f_{ocs} K_{oc} \qquad (7\ 43)$$

$$K_{pB} = 1\ 0\ K_{oc} \qquad (7\ 44)$$

where

K_{oc} = organic carbon partition coefficient L_w/kg_{oc}

f_{ocs} = organic carbon fraction of sediment

1 0 = organic carbon fraction of DOC

Option 3 Computation of the Organic Carbon Partition Coefficient

Correlation of K_{oc} with the water solubility of the chemical or the octonal/water partition coefficient of the chemical has yielded successful predictive tools for incorporating the hydrophobicity of the chemical in an estimate of its partitioning If no log K_{oc} values are available, one is generated internally using the following correlation with the octanol-water partition coefficient K_{ow} (L_w/L_{oc})

$$\log K_{oc} = a_o + a_1 \log K_{ow} \qquad (7\ 45)$$

where a_o and a_1 are typically considered to be log 0 6 and 1 0, respectively Once the value of K_{oc} is determined, the computation of the partition coefficient proceeds as in Option 2

Option 4 Computation of Solids Dependant Partitioning

The value of the partition coefficient is dependent on numerous factors in addition to the fraction organic carbon of the sorbing particles Of these, perhaps the most potentially significant and the most controversial is the effect of particle concentration which was first presented by O'Connor and Connolly (1980) Based on empirical evidence O'Connor and Connolly concluded that the partition coefficient was inversely related to the solids concentration Much research has been conducted to prove or disprove this finding At present the issue remains contentious A particle interaction model has been proposed (Di Toro, 1985) which describes the effects of particle concentration This model was shown to be in conformity with observations for a large set of adsorption-desorption data At present, this should be considered an empirical relationship The equation defining partition coefficient is

$$K_{ps} = \frac{K_{ps0}}{1 + M_s K_{ps0}/\nu_x} \qquad (7\ 46)$$

where

K_{ps0} = limiting partition coefficient with no particle interaction (f_{ocs} K_{oc} for neutral organic chemicals)

M_s = solids concentration kg/L

υ_y = ratio of adsorption to particle-induced desorption rate

Di Toro found that υ_y was of order 1 over a broad range of chemical and solids types This formulation has been included in TOXI5 If υ_x is specified to be 1 0, then TOXI5 will predict a maximum particulate fraction in the water column of 0 5 for all hydrophobic chemicals ($K_{pso}M_s > 10$)

Implementation

Table 7 6 TOXI5 Sorption Data

Description	Notation	Common Range	S I Units
Suspended sediment concentration	m_s	10-100	mg/L
Benthic sediment concentration	M_B	0 5-2	kg/L
Dissolved organic carbon	DOC B	0-10	mg/L
Partition coefficient, phase i	K_{pi}	$10\ ^{1}$-10^{5}	L/kg
Lumped metal distribution coefficient	K_D	10^{0}-10^{5}	L/kg
Octanol-water partition coefficient	K_{ow}	10^{0}-10^{6}	-
Organic carbon fraction, phase i	f_{oci}	0 005-0 5	-
Particle interaction parameter	υ_x	1-10^{12}	-

TOXI5 data specifications for sorption are summarized in Table 7 6 For each chemical modeled, up to 20 partition coefficients are defined representing the five species of chemical (neutral plus four ionic) and the four sorbants (DOC and three types of solids) Normally only a subset of these would be used, as defined by those species and solids being modeled Sorption of the neutral chemical to DOC and the solids is defined by the f_{oc} of the sorbant (assumed to be 1 for DOC), the octanol-water partition coefficient of the chemical (K_{ow}) the user defined relationship between K_{ow} and K_{oc}, and the particle

Table 7 7 TOXI5 Constants for Sorption Reactions

VARIABLE	C_1	C_2	C_3	DEFINITION
LKOW	84	684	1284	Log_{10} octanol-water partition coefficient
LKOC	101	701	1301	Log_{10} organic carbon partition coefficient
A0	102	702	1302	Intercept in the K_{ow} - K_{oc} correlation
A1	103	703	1303	Slope in the K_{ow} - K_{oc} correlation
NUX_1	106	706	1306	Solids dependent partitioning parameter
$PIXC_{1\ 1}$	111	711	1311	Solids independent (limiting) partition coefficient to solids 1
$PIXC_{2\ 1}$	116	716	1316	Solids independent (limiting) partition coefficient to solids 2
$PIXC_{3\ 1}$	121	721	1321	Solids independent (limiting) partition coefficient to solids 3

interaction parameter ν_x values for each species The input ionic species partition coefficients are used as the limiting partition coefficients in equation 7 40 Constant numbers for the different coefficient options are given in Table 7 7

Option 1 Measured Partition Coefficients

For each chemical simulated, separate partition coefficients may be entered for sorption of the neutral molecule and up to 4 ionic species onto each of the three possible solids types and DOC The partition coefficient is input in units of L/kg_s (not in log units) If a partition coefficient is specified it will be used regardless The user is referred to Chapter 6 for details on directly specifying partition coefficients

Solids Partition Coefficient, L/kg-- The user may directly specify partition coefficients to solids using constant PIXC Constant numbers for sorption of the neutral molecule are given in Table 7 7 Constant numbers for sorption of ionic species are given in Part B of this document

DOC Partition Coefficient-- The user may specify partition coefficients for sorption of ionic species to DOC using constant PIDOC Constant numbers are given in Part B of this document For sorption of the neutral molecule, the organic carbon partition coefficient is used

Option 2 Input of Organic Carbon Partition Coefficient

Under this option the user inputs the log (base 10) of the organic carbon partition coefficient (K_{oc}) In addition, the user should also input the fraction organic carbon for each of the solids types simulated The fraction organic carbon for dissolved organic carbon is assumed to be 1 0 The fraction organic carbon and dissolved organic carbon concentration are model parameters, which may be specified for each model segment If a value for the partition coefficient (K_p, Option 1) is input, then K_{oc} will not be used

Organic Carbon Partition Coefficient, L/kg-- The user may specify the $\log_{10}$ of the organic carbon partition coefficient using constant LKOC Constant numbers are given in Table 7 7

Fraction Organic Carbon-- The user should specify the segment variable fraction organic carbon for each solids type simulated using parameters FOC(I,1), FOC(I,2), and FOC(I,3) Parameter numbers for solids 1, 2, and 3 are 7, 8, and 9, respectively

Dissolved Organic Carbon, mg/L-- The user may specify segment variable dissolved organic carbon concentrations using parameter 6, DOC

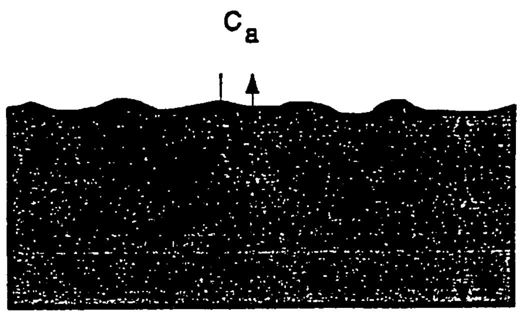
Option 3 Computation of the Organic Carbon Partition Coefficient

Under this option the user allows the model to compute the K_{oc} from a specified octanol water partition coefficient (K_{ow}) The model then computes the K_{oc} using equation 7 39 This option will not be used if values for the log (K_{oc}) are input

Octanol-Water Partition Coefficient, L_w/L_o-- The user may specify the $\log_{10}$ of the octanol-water partition coefficient using constant LKOC Constant numbers are given in Table 7 7

Correlation Coefficients-- The user should specify correlation coefficients relating K_{ow} with K_{oc} using constants A0 and A1 A0 and A1 are the intercept and the slope in the correlation described by equation 7 39 Default values are log 0 6 and 1 0, respectively If these constants are not entered then, the correlation becomes K_{oc} = 0 6 K_{ow} Constant numbers are

VOLATILIZATION



$$\frac{\partial C_W}{\partial t} = -\frac{k_V}{D}\left(C_W - \frac{C_a}{H/RT}\right)$$

C_w - Dissolved Concentration In Water, μg/L
C_a - Concentration In Air, μg/L
H - Henry's Law Constant, atm/M
R - Gas Constant (8 206x10^{-5}), atm/M K
T - Water Temperature, K
D - Depth, m
k_v - Rate Constant, m/day (conductivity)

Figure 7 2 Volatilization reaction

given in Table 7 7

Fraction Organic Carbon-- The user should specify the segment variable fraction organic carbon for each solids type simulated using parameters FOC(I,1), FOC(I,2), and FOC(I,3) Parameter numbers for solids 1, 2, and 3 are 7, 8, and 9, respectively

Dissolved Organic Carbon, mg/L-- The user may specify segment variable dissolved organic carbon concentrations using parameter 6, DOC

Option 4 Solids Dependant Partitioning

The user may include the effect of solids concentration on adsorption by using a value of $\boldsymbol{\upsilon}_x$ of order 1 (see Di Toro, 1985 for more detail) If the user does not provide an input value for $\boldsymbol{\upsilon}_x$, the default value will eliminate any solids effect on the partition coefficient Since collision induced desorption is only expected to occur in the water column, solids dependant partitioning is only computed for water column segments (where porosity is greater that 0 99) In addition to the partical interaction parameter, the user must provide for a partition coefficient following option 1 2 or 3 described above

Particle Interaction Parameter-- The user may implement solids dependent partitioning by specifying an appropriate value for constant NUX A value of order 1 will cause the input partition coefficient to decrease with increasing suspended solids following equation 7 40 Larger values of NUX will reduce the solids effect on partitioning The default value of 10^{12} effectively eliminates this behavior Constant numbers for the solids effect on the neutral molecule are given in Table 7 7 Constant numbers for the solids effect on sorption of ionic species are given in Part B of this documentation

7 5 VOLATILIZATION

Introduction

Volatilization is the movement of chemical across the air-water interface as the dissolved neutral concentration attempts to equilibrate with the gas phase concentration Equilibrium occurs when the partial pressure exerted by the chemical in solution equals the partial pressure of the chemical in the overlying atmosphere The rate of exchange is proportional to the gradient between the dissolved concentration and the concentration in the overlying atmosphere and the conductivity across the interface of the two fluids The conductivity is influenced by both chemical properties (molecular weight, Henry's Law constant) and environmental conditions at the air-water interface (turbulence-controlled by wind speed, current velocity, and water depth)

Overview of TOXI5 Volatilization

The dissolved concentration attempts to equilibrate with the gas phase concentration, as illustrated in Figure 7 2 and given by

$$\frac{\partial C}{\partial t}\bigg|_{volat} = \frac{K_v}{D}\left(f_d C - \frac{C_a}{\frac{H}{RT_K}}\right) \tag{7 47}$$

where

K_v = the transfer rate, m/day
D = segment depth, m
f_d = fraction of the total chemical that is dissolved,
C_a = atmospheric concentration, ug/L
R = universal gas constant, 8 206x10^{5} atm-m^3/mole °K
T_K = water temperature, °K
H = Henry's law coefficient for the air-water partitioning of the chemical, atm-m^3/mole

Equilibrium occurs when the dissolved concentration equals the partial pressure divided by Henry's Law Constant

In TOXI5 the dissolved concentration of a chemical in a surface water column segment can volatilize at a rate determined by the two-layer resistance model (Whitman, 1923) The two-resistance method assumes that two stagnant films are bounded on either side by well mixed compartments Concentration differences serve as the driving force for the water layer diffusion Pressure differences drive the diffusion for the air layer From mass balance considerations it is obvious that the same mass must pass through both films, thus the two resistances combine in series, so that the conductivity is the reciprocal of the total resistance

$$K_v = (R_L + R_G)^{-1} = \left[K_L^{-1} + \left(K_G \frac{H}{RT_K}\right)^{-1}\right]^{-1} \tag{7 48}$$

where

R_L = liquid phase resistance, day/m
K_L = liquid phase transfer coefficient, m/day
R_G = gas phase resistance day/m
K_G = gas phase transfer coefficient, m/day

There is actually yet another resistance involved, the transport resistance between the two interfaces, but it is assumed to be negligible This may not be true in two cases very turbulent conditions and in the presence of surface active contaminants Although this two-resistance method, the Whitman model, is rather simplified in its assumption of uniform layers it has been shown to be as accurate as more complex models

The value of K_v, the conductivity, depends on the intensity of turbulence in a water body and in the overlying atmosphere Mackay and Leinonen (1975) have discussed conditions under which the value of K_v is primarily determined by the intensity of turbulence in the water As the Henry's Law coefficient increases the conductivity tends to be increasingly influenced by the intensity of turbulence in water As the Henry's Law coefficient decreases the value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence

Because Henry s Law coefficient generally increases with increasing vapor pressure of a compound and generally decreases with increasing solubility of a compound, highly volatile low solubility compounds are most likely to exhibit mass transfer limitations in water and relatively nonvolatile high solubility compounds are more likely to exhibit mass transfer limitations in the air Volatilization is usually of relatively less magnitude in lakes and reservoirs than in rivers and streams

In cases where it is likely that the volatilization rate is regulated by turbulence level in the water phase, estimates of volatilization can be obtained from results of laboratory experiments As discussed by Mill et al (1982), small flasks containing a solution of a pesticide dissolved in water that have been stripped of oxygen can be shaken for specified periods of time The amount of pollutant lost and oxygen gained through volatilization can be measured and the ratio of conductivities (KVOG) for pollutants and oxygen can be calculated As shown by Tsivoglou and Wallace (1972), this ratio should be constant irrespective of the turbulence in a water body Thus if the reaeration coefficient for a receiving water body is known or can be estimated and the ratio of the conductivity for the pollutant to reaeration coefficient has been measured, the pollutant conductivity can be estimated

The input computed volatilization rate constant is for a temperature of 20°C It is adjusted for segment temperature using the equation

$$K_{v\,T} = K_{20}\,\theta^{T-20} \qquad (7\ 49)$$

where

θ_v = temperature correction factor
T = water temperature, 蚓

Directly input volatilization rates are not temperature adjusted

<u>Computation of the Transfer Rates</u>

There have been a variety of methods proposed to compute the liquid (K_L) and gas phase (K_G) transfer coefficients, several of which are included in TOXI5 The particular method to be employed is identified by the model through the user's selection of one of six volatilization options, each of which is briefly described below

Volatilization Option 1

This option allows the use of measured volatilization rates The rates (K_v, m/day) are input as a parameter (which may be varied by segments) and may be time variable

Volatilization Option 2

This option allows the user to input an oxygen reaeration constant which is then adjusted to represent the liquid film transfer constant for the particular chemical The adjustment is made in one of two ways First, the user may input a measured ratio of oxygen to chemical exchange so that the rate (K_L) is computed from

$$K_L = K_a \quad K_{vo} \qquad (7\ 50)$$

where

K_a = reaeration velocity, m/day
K_{vo} = ratio of volatilization rate to reaeration rate

If K_{vo} is not provided, TOXI5 will compute the ratio based on the molecular weights of O_2 and the that of the chemical as shown below

$$K_L = K_a \sqrt{32/M_w} \qquad (7\ 51)$$

where M_w = molecular weight of the chemical, g/mole

Under this option the gas transfer rate (K_G) is calculated using O'Conner's method (see Option 4)

Volatilization Option 3

If this option is specified, the liquid film transfer coefficient will be computed as in Option 2 However, the gas film transfer coefficient will be computed using Mackay's method (see Option 5)

Volatilization Option 4

The liquid and gas film transfer coefficients computed under this option vary with the type of waterbody The type of waterbody is specified to the water as one of the volatilization constants and can either be a flowing stream, river or estuary or a stagnant pond or lake The primary difference is that in a flowing waterbody the turbulence is primarily a function of the stream velocity, while for stagnant waterbodies wind shear may dominate The formulations used to compute the transfer coefficients vary with the waterbody type as shown below

a) Flowing Stream, River or Estuary For a flowing system (type 0) the transfer coefficients are controlled by flow induced turbulence For flowing systems, the liquid film transfer coefficient (K_L) is computed using the Covar method (Covar 1976) in which the equation used varies with the velocity and depth of the segment First the transfer coefficient for dissolved oxygen is computed using the formulations provided below and then K_L calculated from equation 7.44 or 7.45

For segments with depths less than 0.61 m the Owens formula is used to calculate the oxygen reaeration rate

$$K_a = 5.349 \frac{u^{0.67}}{D^{0.85}} \tag{7.52}$$

where
u = velocity of the water m/s
D = segment depth, m

For segments with a velocity less than 0.518 m/s or a depth (m) greater than 13.584 $u^{2.9135}$, the O'Connor-Dobbins formula is used

$$K_L = \left(\frac{D_w u}{D}\right)^{0\ 5}\ 8\ 64\ \ 10^4 \qquad (7\ 53)$$

where D_w is the diffusivity of the chemical in water (m^2/s), computed from

$$D_w = \frac{22\ \ 10^{-9}}{M_w^{2/3}} \qquad (7\ 54)$$

In all other cases, the Churchill formula is used to calculate reaeration rate

$$K_a = 5\ 049 \frac{U^{0\ 969}}{D^{0\ 673}} \qquad (7\ 55)$$

The gas transfer coefficient (K_G) is assumed constant at 100 m/day for flowing systems

b) Stagnant Lake or Pond For a stagnant system (type 0) the transfer coefficients are controlled by flow induced turbulence For flowing systems, the liquid film transfer coefficient (K_L) is computed using the O'Connor equations

$$K_L = u^{*}\left(\frac{\rho_a}{\rho_w}\right)^{0\ 5}\ \frac{\kappa^{0\ 33}}{\lambda_2}\ S_{cw}^{-0\ 67} \qquad (7\ 56)$$

$$K_G = u\ \ \frac{\kappa^{0\ 33}}{\lambda_2}\ Sc_a^{-0\ 67} \qquad (7\ 57)$$

where u is the shear velocity (m/s) computed from

$$u\ \ = C_d^{0\ 5}\ W_{10} \qquad (7\ 58)$$

where

C_d = drag coefficient (0 0011)
W_{10} = wind velocity 10 m above water surface m/sec

ρ_a = density of air internally calculated from air temperature, kg/m^3

ρ_w = density of water, internally calculated from water temperature, kg/m^3

κ = von Karmen's constant (0 74)

λ_2 = dimensionless viscous sublayer thickness (4)

S_{ca} and S_{cw} are air and water Schmidt Numbers, computed from

$$S_{ca} = \frac{\mu_a}{\rho_a D_a} \qquad (7\ 59)$$

$$S_{cw} = \frac{\mu_w}{\rho_w D_w} \qquad (7\ 60)$$

where

D_a = diffusivity of chemical in air m^2/sec

D_w = diffusivity of chemical in water, m^2/sec

μ_a = viscosity of air, internally calculated from air temperature, kg/m-sec

μ_w = viscosity of water, internally calculated from water temperature, kg/m-sec

The diffusivity of the chemical in water is computed using Equation 7 48 while the diffusivity of the chemical in air (D_a, m^2/sec) is computed from

$$D_a = \frac{1\ 9\ \ 10^{-4}}{M_w^{2/3}} \qquad (7\ 61)$$

Thus K_G is proportional to wind and inversely proportional to molecular weight to the 4/9 power

Volatilization Option 5

As with Option 4 the liquid and gas film transfer coefficients computed under this option vary with the type of waterbody The type of waterbody is specified to the water as one of the volatilization constants and can either be a flowing stream, river or estuary or a stagnant pond or lake The primary difference is that in a flowing waterbody the turbulence is primarily a function of the stream velocity, while for stagnant waterbodies wind shear may dominate. The formulations used to compute the transfer coefficients vary with the waterbody type as shown below.

a. Flowing Stream, River or Estuary. The liquid and gas film transfer coefficients for flowing waterbodies are computed identically to those described under Option 4.

b) Stagnant Pond or Lake. Under this option, the liquid and gas film transfer coefficients are computed using formulations described by Mackay (1985). The Mackay equations are:

$$K_L = 10^{-6} + 0.00341\, u^*\, Sc_w^{-0.5} \qquad u^* > 3\ m/s \tag{7.62}$$

$$K_L = 10^{-6} + 0.0144\, u^{*2.2}\, Sc_w^{-0.5} \qquad u^* < 3\ m/s \tag{7.63}$$

$$K_G = 10^{-3} + 0.0462\, u^*\, Sc_a^{-0.67} \tag{7.64}$$

Implementation

Although there are many calculations involved in determining volatilization, most are performed internally using a small set of data. TOXI5 volatilization data specifications are summarized in Table 7.8. Not all of the constants are required. If Henry's Law constant is unknown, it will be calculated internally from vapor pressure and solubility (provided in input). If K_{v_o} is not measured, it will be calculated internally from molecular weight and specified or computed liquid film transfer coefficients. Volatilization is only allowed for surficial water column segments as identified by the segment type specified in input. The segment types are: 1) Surface water segments (Type 1), 2) Subsurface water segments (Type 2), Surficial sediment segments (Type 3), and 4) subsurface sediment segments (Type 4).

Transformation input parameters that must be specified by the user are given below for each volatilization option. Constant numbers are listed in Table 7.9. Three constants should be input for all volatilization options: the volatilization option number, Henry's Law Constant and the atmospheric chemical concentration. Segment depths (from Data Group C) must be specified.

Table 7 8 TOXI5 Volatilization Input

Description	Notation	Range	Units
Measured or calibrated conductance	K_v	0 6-25	m/day
Henry's Law Constant	H	10^{7}-10^{1}	atm/mole
Concentration of chemical in atmosphere	C_a	0-1000	痢/L
Molecular weight	M_w	10-10^3	g/mole
Reaeration coefficient (conductance of oxygen)	K_a	0 6-25	m/day
Experimentally measured ratio of volatilization to reaeration	k_{vo}	0-1	
Current velocity	u_x	0-2	m/sec
Water depth	D	0 1-10	m
Water temperature	T	4-30	蚓
Wind speed 10 m above surface	W_{10}	0-20	m/sec

Volatilization Option-- The user should chose the volatilization option using constant XV Specifying a value of 0 will prevent volatilization from occuring Values of 1 - 5 will invoke volatilization options 1 - 5 as outlined in the text above (1) volatilization rates are input directly, (2) volatilization is computed from input reaeration rate constants and O'Connor's equation for gas transfer, (3) volatilization is computed from input reaeration rate constants and MacKay's equation for gas transfer (4) in flowing systems, volatilization is computed using reaeration rates calculated from Covar's method and a gas transfer rate of 100 m/day, in quiescent systems volatilization is computed from O Connor's equations for liquid and gas transfer, (5) in flowing systems, volatilization is computed using reaeration rates calculated from Covar's method and a gas transfer rate of 100 m/day in quiescent systems, volatilization is computed from MacKay's equations for liquid and gas transfer

Henry's Law Constant, atm-m^3/mole-- The user should specify Henry's Law constant for air-water partitioning of the chemical using constant HENRY

Atmospheric Concentration, ug/L-- The user should specify

Table 7 9 TOXI5 Constants for Volatilization Reactions

VARIABLE	C_1	C_2	C_3	DEFINITION
WTYPE	2	2	2	Water body type (0 = flowing, 1 = quiescent)
AIRTMP	5	5	5	Multiplier for air temperature time function
ATMOS	8	608	1208	Atmospheric concentration of chemical, ug/L
MOLWT	81	681	1281	Molecular weight of chemical
SOLG	82	682	1282	Solubility of chemical in water, mg/L
VAPRG	83	683	1283	Vapor pressure of chemical, torr
XV	136	736	1336	Volatilization option 0 = none 1 = measured 2 = measured reaeration + O'Connor, 3 = measured reaeration + MacKay, 4 = calculated by O'Connor, 5 = calculated by MacKay
HENRY	137	737	1337	Henry's Law constant, atm-m^3/mole
KLT	138	738	1338	Volatilization temperature correction factor
KVOG	139	739	1339	Measured ratio of volatilization to reaeration rate

the mean atmospheric concentration of chemical using constant ATMOS If this concentration is 0, then volatilization will always cause a loss of chemical from the water body

Volatilization Option 1

In this option, variable volatilization rate constants can be input directly

Volatilization Rates, m/day-- When XV is set to 1 the user may then input segment and time variable volatilization rates using parameter 5 REAR, and time function 12, REARN The product of spatially-variable REAR and time-variable REARN gives the segment and time specific volatilization rate constants used by TOXI5 These volatilization values are not modified by a temperature function

Volatilization Option 2

In this option, volatilization rates are calculated from user-input reaeration rate constants and O'Connor's method for gas transfer Input data required for option 2 are listed below For flowing systems, wind speed and air temperature are not used and may be omitted

Water Body Type-- The user should specify the water body type using constant WTYPE A value of 0 indicates a flowing water body, such as a stream, river, or estuary A value of 1 indicates a quiescent water body, such as a pond, reservoir, or lake

Reaeration Rates, m/day-- When XV is set to 2, the user may then input segment and time variable reaeration rates using parameter 5, REAR, and time function 12, REARN The product of spatially-variable REAR and time-variable REARN gives the segment and time specific reaeration rate constants used by TOXI5 These reaeration values are not modified by a temperature function

Ratio of Volatilization to Reaeration-- The user may specify an experimentally-measured ratio of volatilization to reaeration using constant KVOG If this constant is not given, the ratio will be calculated from molecular weight

Molecular Weight g/mole-- The user may specify the molecular weight using constant MOLWT This constant is used to calculate the ratio of volatilization to reaeration if an experimentally-measured value is not provided It is also used in the calculation of diffusivities

Wind Speed, m/sec-- The user may specify the segment and time variable wind speed using parameter 4, WVEL, and time function 9, WINDN The product of spatially-variable WVEL and time-variable WINDN gives the segment and time specific reaeration rate constants used by TOXI5 Wind speed should be measured at 10 m height above the water surface

Air Temperature, [illegible]-- The user may specify time-variable air temperature using constant AIRTMP and time function 13 AIRTMPN The ambient air temperature is calculated as the product of AIRTMP and AIRTMPN For a constant air temperature, AIRTMPN can be omitted For variable air temperatures, the user should set AIRTMP to 1 0 and input a series of air temperature versus time values via AIRTMPN

Volatilization Option 3

In this option, volatilization rates are calculated from user-input reaeration rate constants and MacKay's method for gas transfer Input data required for the same as for option 2, listed above For flowing systems, wind speed and air temperature are not used and may be omitted

Volatilization Option 4

In this option, volatilization rates in flowing systems are calculated using reaeration rates calculated from Covar's method and a gas transfer rate of 100 m/day In quiescent systems, volatilization is computed from O'Connor's equations for liquid and gas transfer Input data required for option 4 are listed below For flowing systems, wind speed and air temperature are not used and may be omitted For quiescent systems, water velocity may be omitted

Water Velocity, m/sec-- Variable current velocities are calculated from flow using hydraulic geometry coefficients as described in Chapter 2 For most situations, no further input is required from the user If an estuary is being simulated under tidal-average conditions, however, the net flows do not provide realistic ambient water velocities for use in volatilization calculations In this case, the user should enter time and segment variable water velocities using parameter 1, VELFN and time functions 5-8, VELN(1-4)

The parameter VELFN indicates which velocity function will be used by the model for each segment Values of 1 0, 2 0, 3 0, or 4 0 will call time functions VELN(1), VELN(2) VELN(3) and VELN(4), respectively Water velocities should then be entered via these time functions as a series of velocity versus time values

Water Body Type-- see Option 2 above

Ratio of Volatilization to Reaeration-- see Option 2 above

Molecular Weight g/mole-- see Option 2 above

Wind Speed, m/sec-- see Option 2 above

Air Temperature, C-- see Option 2 above

Volatilization Option 5

In this option, volatilization rates in flowing systems are calculated using reaeration rates calculated from Covar s method and a gas transfer rate of 100 m/day In quiescent systems, volatilization is computed from MacKay's equations for liquid and gas transfer Input data required for option 5 are the same as for option 4 above For flowing systems, wind speed and air temperature are not used and may be omitted For quiescent systems, water velocity may be omitted

7 6 HYDROLYSIS

Introduction

Hydrolysis, or reaction of the chemical with water, is known to be a major pathway for degradation of many toxic organics Hydrolysis is a reaction in which cleavage of a molecular bond of the chemical and formation of a new bond with either the hydrogen or the hydroxyl component of a water molecule occurs Hydrolytic reactions are usually catalyzed by acid and/or base and the overriding factor affecting hydrolysis rates at a given

HYDROLYSIS

Neutral $C + H_2O \longrightarrow P + P'$

Acid Catalysis $C + H_2O \xrightarrow{H^+} P + P'$

Base Catalysis $C + H_2O \xrightarrow{OH} P + P'$

EXAMPLE

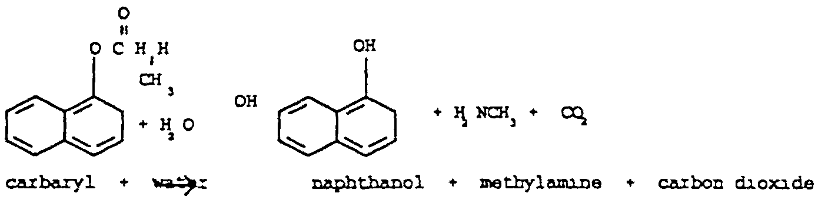


Figure 7 3 Hydrolysis reactions

temperature is generally hydrogen or hydroxide ion concentration (Wolfe, 1980) An example reaction is shown in Figure 7 3 The reaction can be catalyzed by hydrogen ions or proceed by consuming hydroxide ions Figure 7 4 illustrates the effects of base hydrolysis on carbaryl, neutral hydrolysis on chloromethane, and acid and base hydrolysis on 2,4-D

Overview of TOXI5 Hydrolysis Reactions

Hydrolysis may be simulated by TOXI5 using simple decay Alternatively, hydrolysis can be simulated using rates that are first order for the neutral chemical and second order for its ionic forms The second order rates are pH and temperature dependant

Option 1 First Order Hydrolysis

Under this option, the user inputs a first order rate constant for either neutral, alkaline, or acid hydrolysis The first order rate term constant is then applied to the total chemical concentration (see Section 6 3)

Option 2 Second Order Hydrolysis

Under this option, hydrolysis by specific-acid-catalyzed, neutral, or base pathways is considered for the various species and phases of each chemical The reactions are first order for the neutral chemical and second order for the acidic or basic forms of the chemical

$$K_{HN} = \sum_i \sum_j k_{nij} \, f_{ij} \qquad (7\ 65)$$

$$K_{HH} = \sum_i \sum_j k_{aij} \, [H^+] \, f_{ij} \qquad (7\ 66)$$

$$K_{HOH} = \sum_i \sum_j k_{bij} \, [OH^-] \, f_{ij} \qquad (7\ 67)$$

where

K_{HN} = net neutral hydrolysis rate constant, day

K_{HH} = net acid catalyzed hydrolysis rate constant day^{1}

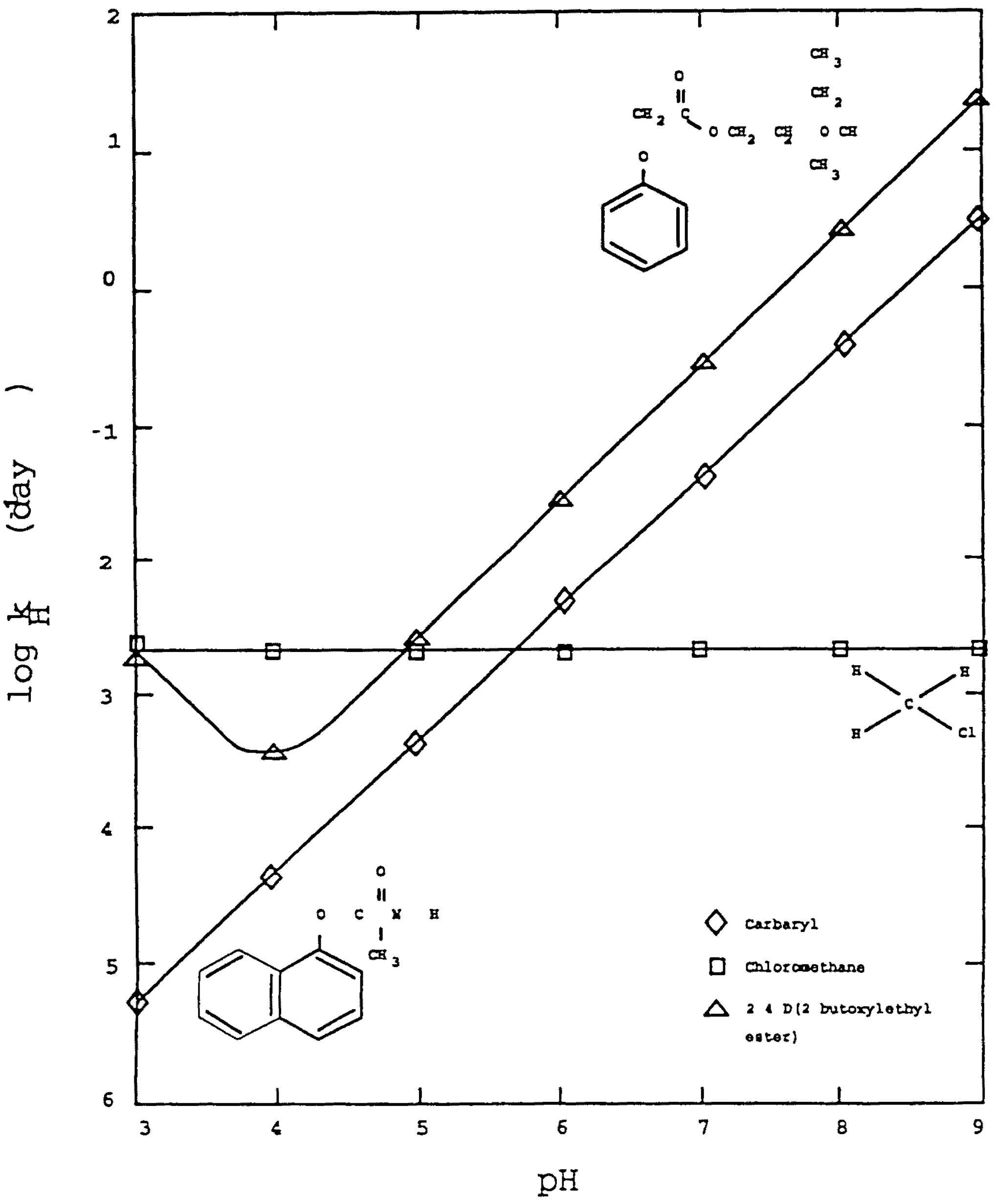


Figure 7 4 pH dependence of hydrolysis rate constants

K_{HOH} = net base catalyzed hydrolysis rate constant, day ^{1}

k_{aij} k_{bij} = specific acid catalyzed and base rate constants for ionic specie i in phase j, respectively, molar ^{1} day ^{1}

k_{nij} = neutral rate constant for ionic specie i in phase j, day ^{1}

f_{ij} = fraction of chemical as ionic specie i in phase j

The rates are also affected by temperature TOXI5 adjusts the rates using the temperature-based Arrhenius function

$$k(T_k) = k(T_R)\ \exp[1000\ E_{aH}(T_K - T_R)/(RT_k\ T_R)] \qquad (7\ 68)$$

where

T_K = water temperature, 袁

T_R = reference temperature for which reaction rate is reported, 袁

E_{aH} = Arrhenius activation energy for hydrolysis reaction kcal/mole 袁

R = 1 99 cal/mole 袁

1000 = cal/kcal

Implementation

TOXI5 hydrolysis data specifications are summarized in Table 7 10 In addition the simple first order rates may be specified as described under Option 1 and the section on simple TOXI5 reactions If no hydrolysis data are input, then the effect of hydrolysis will not be included in simulations

Option 1

Under this option, the user inputs one or more of the following an acid, neutral, and base hydrolysis rate constant

First-Order Hydrolysis Rate Constants, day ^{1}-- The user may input overall base, neutral, and acid hydrolysis rate constants

Table 7 10 TOXI5 Hydrolysis Data

Description	Notation	Range	Units
Negative log of hydrogen ion activity [H^{+}]	pH	5-9	-
Acid hydrolysis rate constant for specie i, phase j	k_{HAij}	$0-10^{7}$	
Neutral hydrolysis rate constant for specie i, phase j	k_{HNij}	$0-10^{2}$	day ^{1}
Base hydrolysis rate constant for specie i, phase j	k_{HBij}	$0-10^{7}$	
Water temperature	T	4-30	蚓
Activation energy for hydrolysis reaction for specie i	E_{aHi}	15-25	

using constants 181, 182 and 183 for chemical 1 constants 781, 782 and 783 for chemical 2, and constants 1381 1382 and 1383 for chemical 3 The rates are first order, and are applied to the total chemical If any one of these first order rates are specified in input they will be used regardless of whether other hydrolysis constants are specified

Option 2

Under this option the reaction coefficients can be specified as constants If the chemical simulated does not ionize (as controlled by input of the ionization constants), then acid, base and neutral hydrolysis constants may be input for the dissolved, DOC sorbed and sediment sorbed phases of the chemical as summarized in Table 7 11 If ionization of the chemical is allowed, then constants may be input for the dissolved DOC sorbed and sediment sorbed phases of each ionic specie simulated In addition, the pH must be supplied in order to compute acid and base hydrolysis The pH is input as a parameter, which must be specified for each model segment and may be constant or time variable Separate pH time functions may be specified for surface water and benthic segments

If the user wants TOXI5 to adjust the rates based on temperature, then non-zero activation energies should be

Table 7 11 TOXI5 Constants for Hydrolysis Reactions

PHASE "i" or REACTION "k"	C$_1$	C$_2$	C$_3$	INPUT VARIABLE
all	184	784	1384	Reference Temperature TREFH 蚓
aqueous	186	786	1386	Alkaline Hydrolysis KH2O$_{1\ i\ 1}$ M ^{1}day ^{1}
DOC	191	791	1391	
sediment	196	796	1396	
aqueous	201	801	1401	Neutral Hydrolysis KH2O$_{2\ i\ 1}$ day ^{1}
DOC	206	806	1406	
sediment	211	811	1411	
aqueous	216	816	1416	Acid Hydrolysis KH2O$_{3\ i\ 1}$ M ^{1}day ^{1}
DOC	221	821	1421	
sediment	226	826	1426	
Alkaline	231	831	1431	Activation Energy E$_{ak}$, kcal/mole 袁
Neutral	236	836	1436	
Acid	241	841	1441	

specified which will invoke the temperature-based Arrhenius function Activation energies may be specified for each ionic specie and each hydrolysis reaction (acid, neutral, base) simulated If no activation energies are given, then rates constants will not be adjusted to ambient water temperatures

Base Hydrolysis Rate Constants, M ^{1}day ^{1}-- The user may specify second order base hydrolysis rate constants for each phase (dissolved DOC-sorbed, and sediment-sorbed) and each ionic specie using constant KH20 Constant numbers for the neutral molecule are summarized in Table 7 11 KH20$_{1\ 1\ 1}$ refers to the dissolved neutral chemical, KH20$_{1\ 2\ 1}$ refers to the DOC-sorbed neutral chemical KH20$_{1\ 3\ 1}$ refers to the sediment-sorbed neutral chemical Constant numbers for the ionic species are given in Part B of this document

Neutral Hydrolysis Rate Constants, day ^{1}-- The user may specify first order neutral hydrolysis rate constants for each phase (dissolved, DOC-sorbed, and sediment-sorbed) and each ionic specie using constant KH20   Constant numbers for the neutral molecule are summarized in Table 7 11 $KH20_{2\ 1\ 1}$ refers to the dissolved neutral chemical, $KH20_{2\ 2\ 1}$ refers to the DOC-sorbed neutral chemical, $KH20_{2\ 3\ 1}$ refers to the sediment-sorbed neutral chemical   Constant numbers for the ionic species are given in Part B of this document

Acid-Catalyzed Hydrolysis Rate Constants, $M^{-1}day^{-1}$-- The user may specify second order acid-catalyzed hydrolysis rate constants for each phase (dissolved, DOC-sorbed, and sediment-sorbed) and each ionic specie using constant KH20   Constant numbers for the neutral molecule are summarized in Table 7 11 $KH20_{3\ 1\ 1}$ refers to the dissolved neutral chemical, $KH20_{3\ 2\ 1}$ refers to the DOC-sorbed neutral chemical, $KH20_{3\ 3\ 1}$ refers to the sediment-sorbed neutral chemical   Constant numbers for the ionic species are given in Part B of this document

Arrhenius Activation Energy, kcal/mole-袁-- The user may specify activation energies for each chemical using constant EHOH   Constant numbers are summarized in Table 7 11   If EHOH is omitted or set to 0, hydrolysis rates will not be affected by temperature

Reference Temperature, 蚓-- The user may specify the reference temperature at which hydrolysis rates were measured using constant TREFH   Constant numbers are summarized in Table 7 11   If a reference temperature is not supplied   then a default of 20 蚓 is assumed

pH-- The user may specify time and segment variable pH values using parameter 11, PH, and time functions 10 and 11, PHNW and PHNS   The pH in a water segment will be the product of PH and PHNW   the pH in a benthic segment will be the product of PH and PHNS   For constant pH   the user should enter values via parameter PH   Time functions should be omitted   For time variable pH, the user should enter a series of pH versus time values via PHNW and PHNS   The parameter PH values will then represent the ratio of pH in each segment to the time function

7 7 PHOTOLYSIS

Introduction

Photodegradation (photolysis) is the transformation or degradation of a compound that results directly from the adsorption of light energy   An example of several photochemical pathways is given in Figure 7 5   It is a function of the quantity and wavelength distribution of incident light, the light adsorption characteristics of the compound, and the efficiency at

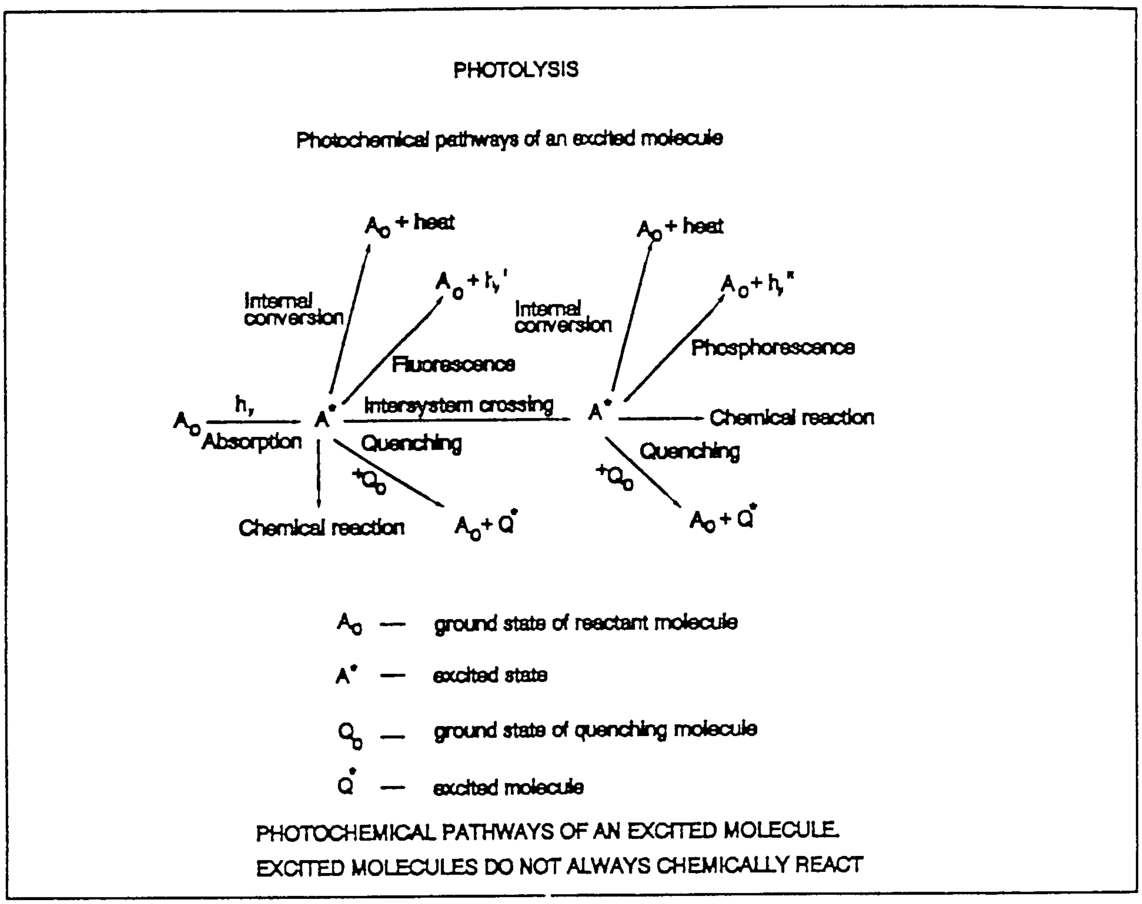


Figure 7 5 Photolysis reactions

which absorbed light produces a chemical reaction Photolysis is classified into two types that are defined by the mechanism of energy absorption Direct photolysis is the result of direct absorption of photons by the toxic chemical molecule Indirect or sensitized photolysis is the result of energy transfer to the toxic chemical from some other molecule that has absorbed the radiation

Overview of TOXI5 Photolysis Reactions

Photolysis is the transformation of a chemical due to absorption of light energy The first order rate coefficient for photolysis can be calculated from the absorption rate and the quantum yield for each ionic specie and phase

$$K_{pG} = \sum_i \sum_j k_{ai} \Phi_{ij} f_{ij} \tag{7 69}$$

where

K_{pG} = first order photolysis rate coefficient at ambient light intensity, day^{1}

k_{ai} = specific sunlight absorption rate for specie i, E/mole-day or (E/L)/(mole/L)/day

Φ_{ij} = reaction quantum yield for specie i in phase j, mole/E

f_{ij} = fraction of chemical as specie i in phase j

The user may specify that the model calculate the first order photolysis rate constant or the user may provide a near water surface rate (for presumed cloudless conditions) If the user-supplied rate constant is representative of conditions at a location other than the water body being modeled the model corrects the rate for the difference in latitude between the two and any difference in cloud cover The options for computing the losses due to photolysis are briefly described below

Photolysis Option 1

Under this option, the photolysis rate is calculated from molar absorptivities calculated light intensity, and quantum yield of the chemical To calculate the rate constant, TOXI5 divides the wavelength spectrum between 280 and 800 nm into 46 intervals For each interval the user must specify a molar absorptivity The light intensity at each of the 46 wavelengths is internally calculated from the location of the water body (i e , latitude), the time of year, and the atmospheric conditions (air mass type, relative humidity, atmospheric turbidity and ozone content, cloudiness) The location and time of year are used to define the light intensity at the outer edge of the atmosphere The atmospheric conditions are used to define the light decay through the atmosphere The light intensities and the molar absorptivities are used with a user defined optical path (d) to calculate the specific sunlight absorption rate The first order rate constant is then calculated using equation 7 63 This calculation was taken directly from EXAMS II (Burns and Cline, 1985) and is based on formulations published by Green Cross and Smith (1980)

The specific sunlight absorption rate is the integral or summation over all bandwidths of the average light multiplied by the molar absorptivity and the optical path

Table 7 12 Wavelength Intervals and Specific Light Extinction Coefficients Used in the Photolysis Calculation Values Taken From EXAMS II (Burns and Cline, 1985)

		Specific Light Extinction Coefficients			
Number	Wavelength	Pure Water 1/m	Chlorophyll L/gm-m	DOC L/mg-m	Solids L/mg-m
1	280 0	0 288	145	7 90	0 34
2	282 5	0 268	138	7 65	0 34
3	285 0	0 249	132	7 41	0 34
4	287 5	0 231	126	7 11	0 34
5	290 0	0 215	120	6 95	0 34
6	292 5	0 194	115	6 73	0 34
7	295 0	0 174	109	6 52	0 34
8	297 5	0 157	106	6 30	0 34
9	300 0	0 141	101	6 12	0 34
10	302 5	0 133	95	5 94	0 34
11	305 0	0 126	90	5 76	0 34
12	307 5	0 119	85	5 57	0 34
13	310 0	0 105	80	5 39	0 34
14	312 5	0 0994	78	5 22	0 34
15	315 0	0 0952	75	5 06	0 34
16	317 5	0 0903	72	4 90	0 34
17	320 0	0 0844	70	4 74	0 34
18	323 1	0 0793	68	4 56	0 34
19	330 0	0 0678	64	4 17	0 34
20	340 0	0 0561	59	3 64	0 34
21	350 0	0 0463	55	3 15	0 34
22	360 0	0 0379	55	2 74	0 34
23	370 0	0 0300	51	2 34	0 34

Table 7 13 Wavelength Intervals and Specific Light Extinction Coefficients Used in the Photolysis Calculation Values Taken From EXAMS II (Burns and Cline, 1985, completed)

		Specific Light Extinction Coefficients			
Number	Wavelength	Pure Water 1/m	Chlorophyll L/gm-m	DOC L/mg-m	Solids L/mg-m
24	380 0	0 0220	46	2 00	0 34
25	390 0	0 0191	42	1 64	0 34
26	400 0	0 0171	41	1 39	0 34
27	410 0	0 0162	39	1 19	0 34
28	420 0	0 0153	38	1 02	0 34
29	430 0	0 0144	35	0 870	0 34
30	440 0	0 0145	32	0 753	0 34
31	450 0	0 0145	31	0 654	0 34
32	460 0	0 0156	28	0 573	0 34
33	470 0	0 0156	26	0 504	0 34
34	480 0	0 0176	24	0 444	0 34
35	490 0	0 0196	22	0 396	0 34
36	503 75	0 0295	19	0 357	0 34
37	525 0	0 0492	14	0 282	0 34
38	550 0	0 0638	10	0 228	0 34
39	575 0	0 0940	8	0 188	0 34
40	600 0	0 244	6	0 158	0 34
41	625 0	0 314	5	0 0	0 34
42	650 0	0 349	8	0 0	0 34
43	675 0	0 440	13	0 0	0 34
44	706 25	0 768	3	0 0	0 34
45	750 0	2 47	2	0 0	0 34
46	800 0	2 07	0	0 0	0 34

$$k_{ai} = \sum_{k} I_{Gk}\, \epsilon_{ki}\, d\ (2303)\ (86400) / (6\ 022 \times 10^{23}) \qquad (7\ 70)$$

where

I_{Gk} = average light intensity of wavelength k photons/cm^2-sec

ϵ_{ki} = decadic molar absorptivity of wavelength k by specie i, L/mole-cm-ln 10

d = ratio of the optical path to the vertical path, cm/cm

2303 = (cm^3/L) (ln 10/ln e)

86400 = sec/day

6 022 x 10^{23} = Avagadro's number, photons/E

Light extinction is calculated with the integrated Beer-Lambert formulation for each wavelength k

$$\frac{I_{Gk}}{I_{ok}} = \frac{1 - \exp(-d\, K_e\, D)}{d\, K_e\, D} \qquad (7\ 71)$$

where

I_{ok} = light intensity of wavelength k just below water surface photons/cm^2-sec

K_e = spatially variable light extinction coefficient, m^{1}

D = depth of water segment, m

I_{ok} is calculated for each wavelength based upon the time of year, latitude, ground elevation, cloud cover, air mass type, relative humidity, atmospheric turbidity, and ozone content The atmospheric characteristics can vary monthly, or be specified as an annual average The value of d the ratio of the optical path to the vertical depth is difficult to compute but a probable best value is 1 19 (Hutchinson Treatis Limnology) However, in the presence of a large concentration of scattering particles, it may approach 2 0 In order to ensure that an improper value is not loaded and used in computations, the input value is checked and set to 1 19 if the input is invalid

The photolysis rate constants for each water column segment are determined from the calculated near-surface rate constant and the rate of light decay in the water column (K_e) The value of K_e is calculated for each wavelength based on a formulation taken from EXAMS II

$$K_e = K_{ew} + \eta_1 \, CHL + \eta_2 \, DOC + \eta_3 \, m \qquad (7\ 72)$$

where

K_{ew} = pure water extinction coefficient 1/m

CHL = phytoplankton chlorophyll concentration, mg/L

DOC = dissolved organic carbon concentration, mg/L

m = solids concentration, mg/L

$\eta 1, \eta 2, \eta 3$ = specific extinction coefficients, L/mg-m

Values of K_{ew} $\eta 1$, $\eta 2$, $\eta 3$ for each of the 46 wavelengths are supplied in the program as data statements in subroutine BEER and are shown in Tables 7 12 and 7 13 Segment average photolysis rate constants are computed for each wavelength and then summed to yield an overall rate

Photolysis Option 2

Under this option a reference surface sunlight absorption rate k_{aRi} (E/mole-day) is input by the user for each specie simulated As with EXAMSII the input rate is then adjusted as shown below

$$k_{ai} = \sum_{i} \sum_{j} k_{aRi} \, I_o \, (I_G/I_o) \, (1-0\ 056\,C) \, X_L \qquad (7\ 73)$$

where

I_o = user specified normalized light intensity time function, which is the ratio of ambient light intensity to the reference light intensity

C = cloud cover (in tenths 0-10)

X_L = latitude correction factor, calculated by

Table 7 14 TOXI5 Photolysis Data

Description	Notation	Range	Units
Observed rate constant for a chemical at reference light intensity I_R	K_{pR}	0 - 10	day ^{1}
Observed sunlight absorption rate for a chemical at reference light intensity I_R	k_{aR}	?	E/mole-day
Reference light intensity causing photolysis rate K_{pR} or absorption rate k_{aR}	I_R	10 ^{7}-2x10 ^{6}	E/cm^{2}-sec
Ratio of surface light intensity to reference light intensity (I_o/I_R)	I_o	0 - 10	-
Light extinction coefficient in water column	K_e	0 1 - 5	m ^{1}
Chlorophyll a concentration	CHL	10 ^{3} - 10 ^{1}	mg/L
Dissolved organic carbon	DOC	0 - 10	mg/L
Depth of water column segment	D	0 1 - 10	m
Reaction quantum yield fraction for specie i in phase j	Φ_{ij}	0 - 0 5	moles/E
Molar absorptivity by wavelength k by specie i	ϵ_{ki}	0 - ?	L/mole-cm-ln 10
Waterbody elevation	ELEVG	0 - 5000	m
Waterbody latitude	L	0 - 90	degrees
Reference latitude	L_o	0 - 90	degrees
Cloud cover, fraction of sky	C_c	0 - 10	tenths
Air type (rural urban, maritime or tropospheric)	AIRTYG	1 - 4	-
Relat[illegible] humidity	RHUMG	0 - 100	percent
Atmospheric turbidity in equivalent aerosol layer thickness	ATURBG	0 - ?	km
Ozone content	OZONEG	0 - ?	cm NTP

$$X_L = \left[\frac{19169\ 65 + 87054\ 63\cos(0\ 039L)}{19169\ 65 + 87054\ 63\cos(0\ 039L_{Rf})}\right] \qquad (7\ 74)$$

where

L = latitude of the waterbody

L_{Rf} = reference latitude at which the surface photolysis rate was measured

The average light intensity attenuation, I_G/I_o, is computed as above from the Beer-Lambert formulation (equation 7 65) Therefore, the light intensity has a value for each model segment ranging from zero to one

The extinction coefficient may be directly specified as a model parameter, which may be varied by model segment If the extinction coefficient is not specified, it is determined from a user-specified wavelength of maximum light absorption for the particular chemical species (neutral, anionic or cationic) using equation 7 66 and the values listed in Tables 7 12 and 7 13 If the wavelength of maximum absorption is outside of the relevant spectral range (280-825 nm) then TOXI5 assumes a wavelength of 300 nm

After adjusting the reference sunlight absorption rate to ambient conditions the first order photolysis rate is computed from these and reaction quantum yields following equation 7 63

Photolysis option 2 is often implemented using reference first order photolysis rate constants rather than reference sunlight absorption rates If reference first order rate constants are input for k_{aRi}, then equation 7 67 calculates k_a as first order rate constants (day^{1}) adjusted to ambient light conditions The overall first order photolysis rate constant is then calculated following equation 7 63 where quantum yields are set to 1 0

Implementation

The TOXI5 photolysis data specifications are summarized in Table 7 14 In addition an overall first-order rate constant may be supplied by the user for each chemical as presented in Chapter 6 If the overall first order rate constant is specified it will be used regardless of other input specifications For the photolysis computations described in this chapter input requirements are described below

Photolysis Option 1

In option 1, TOXI5 computes the sunlight absorption and the surface photolytic decay rate

Photolysis Option-- The user should select the photolysis option using constant XPHOTO 0 = no photolysis, 1 = photolysis rates will be computed from molar absorptivity 2 = photolysis rates will be extrapolated from measured surface rates Use constant numbers 286, 886, and 1486 for chemicals 1, 2, and 3, respectively

Molar Absorptivity, L/mole-cm-ln10-- The user may specify molar absorptivity values for each ionic specie over 46 wavelengths using constant ABS The wavelengths by number are listed in Tables 7 12 and 7 13 Absorptivity values for each ionic specie apply across all phases (aqueous, DOC-sorbed, sediment-sorbed) Constant numbers for the neutral ionic specie are summarized in Table 7 15

Quantum Yield, moles/einstein-- The user may specify reaction quantum yield values for each phase (dissolved DOC-sorbed, sediment-sorbed) and each ionic specie using constant QUANTG Constant numbers for the neutral molecule are summarized in Table 7 15 $QUANTG_{11}$ refers to the dissolved neutral chemical, $QUANTG_{21}$ refers to the DOC-sorbed neutral chemical, $QUANTG_{31}$ refers to the sediment-sorbed neutral chemical

Julian Date-- The user should specify the Julian date for the beginning of the simulation using constant 1 - TO

Elevation, m-- The user should specify the average ground elevation using constant 3 - ELEVG

Table 7 15 Photolysis 1 Constants

VARIABLE	C_1	C_2	C_3
$ABS_{1,L}$	301-346	901 - 946	1501-1546
$QUANTG_{11}$	551	1151	1751
$QUANTG_{21}$	556	1156	1756
$QUANTG_{31}$	561	1161	1761

Latitude, degrees and tenths-- The user should specify the latitude of the waterbody using constant 4 - LATG

Light Option-- Using constant 6 - XLITE, the user has a choice of options controlling how TOXI5 computes and uses light intensity 0 = do not compute light, 1 = compute annual average light intensity, 2 = compute average light intensity for the month indicated by TO, 3 = compute monthly light intensity as a step function

Optical Path-- The user may specify the ratio of the optical path to the vertical depth using constant 7 - DFACG A default value of 1 17 is assumed

Cloud Cover, tenths-- The user should specify the mean monthly or annual average cloud cover using constant CLOUDG Monthly values can be entered using constant numbers 11-22, the annual average can be entered using number 23

Air Type-- The user should specify the mean air mass type using constant AIRTYC Values of 1 2, 3, or 4 will select rural, urban, maritime or tropospheric, respectively Monthly values can be entered using constant numbers 24-35, the annual average can be entered using number 36

Relative Humidity, percent-- The user should specify the mean monthly daylight relative humidity using constant RHUMG Monthly values can be entered using constant numbers 37-48, the annual average can be entered using number 49

Atmospheric Turbidity, km-- The user should specify the mean atmospheric turbidity (in equivalent aerosol layer thickness, km) using constant ATURBG Monthly values can be entered using constant numbers 50-61, the annual average can be entered using number 62

Ozone Content, cm NTP-- The user should specify the mean ozone content (cm NTP) using constant OZONEG Monthly values can be entered using constant numbers 63-74 the annual average can be entered using number 75

Dissolved Organic Carbon, mg/L-- The user may specify segment variable dissolved organic carbon concentrations using parameter 6 - DOC (Group G Record 4 PARAM(I 6))

Chlorophyll a, mg/L-- Time and segment variable phytoplankton chlorophyll *a* concentrations can be specified using parameter 10, CHPHL and time function 14 CHLN If chlorophyll concentrations are to remain constant in time the user should enter segment mean concentrations using parameter CHPHL CHLN should be omitted

The user may enter time-variable chlorophyll *a* concentrations via time function CHLN as a series of concentration versus time values Parameter CHPHL will then represent the ratio of each segment concentration to the time function values   The product of CHPHL and the CHLN function gives the segment and time specific chlorophyll concentrations used by TOXI5   (Group G, Record 4, PARAM(I,10), Group I, Record 2, VALT(14,K)

Photolysis Option 2

In option 2, TOXI5 extrapolates either observed sunlight absorption rates or photolytic decay rates under "reference conditions to ambient conditions   Required input data are described below

Photolysis Option-- The user should select the photolysis option using constant XPHOTO   0 = no photolysis, 1 = photolysis rates will be computed from molar absorptivity, 2 = photolysis rates will be extrapolated from measured surface rates   Use constant numbers 286, 886, and 1486 for chemicals 1, 2, and 3, respectively

Measured Photolysis Rate, day^{-1}-- The user may specify the measured photolysis rate constant under reference conditions using constant KDPG   Values for the neutral molecule of chemicals 1, 2, and 3 can be entered using constants 291, 891, and 1491, respectively   Separate values can be entered for each ionic specie   constant numbers are listed in Part B of this document   If a reference first order rate constant is input, the quantum yield should be set to 1 0

Measured Sunlight Absorption Rate, einstein/mole-day-- The user may specify measured sunlight absorption rates under reference conditions using constant KDPG   Values for the neutral molecule of chemicals 1, 2, and 3 can be entered using constants 291, 891, and 1491, respectively   Separate values can be entered for each ionic specie, constant numbers are listed in Part B of this document   If a reference sunlight absorption rate is input the corresponding quantum yield must be specified

Quantum Yield, moles/einstein-- The user may specify reaction quantum yield values for each phase (dissolved   DOC-sorbed   sediment-sorbed) and each ionic specie using constant QUANTG   Constant numbers for the neutral molecule are summarized in Table 7 15 $QUANTG_{11}$ refers to the dissolved neutral chemical $QUANTG_{21}$ refers to the DOC-sorbed neutral chemical, $QUANTG_{31}$ refers to the sediment-sorbed neutral chemical   Separate values can be entered for each ionic specie, constant numbers are listed in Part B of this document

Reference Latitude, degree and tenths-- The user may specify the latitude at which the reference surface water photolytic rates were measured using constant RFLATG   Values for chemicals 1, 2, and 3 can be entered using constant numbers 288, 888, and

1486, respectively

Maximum Absorption Wavelength, nm-- The user should specify the wavelength of maximum absorption using constant LAMAXG Values for the neutral specie of chemicals 1 2, and 3 can be entered using constants 296, 896, and 1496, respectively Separate values can be entered for each ionic specie, constant numbers are listed in Part B of this document

Latitude, degrees and tenths-- The user should specify the latitude of the waterbody using constant 4 - LATG

Cloud Cover, tenths-- The user should specify the mean monthly or annual average cloud cover using constant CLOUDG Monthly values can be entered using constant numbers 11-22, the annual average can be entered using number 23

Light Intensity-- The user can specify time-variable normalized light intensity (dimensionless) using time function 15, PHTON This function is used to adjust the measured rate constant under controlled reference light intensity to a predicted rate constant under ambient light intensity The default value for this function is 1 0

Light Extinction Coefficient, m^{-1}-- The user can specify segment light extinction coefficients for the photochemically active light using parameter 12, XKE2 When this number is zero the extinction coefficients are calculated from solids, DOC and chlorophyll *a* concentrations for the wavelength of maximum absorption DOC and chlorophyll *a* are specified as model parameters which may vary between segments and over time Their input is describe in the Photolysis Option 1 section above Light is set to zero under ice cover, which is assumed when water temperatures reach 0 °C

7 8 OXIDATION

Introduction

Chemical oxidation of organic toxicants in aquatic systems can be a consequence of interactions between free radicals and the pollutants Free radicals can be formed as a result of photochemical reactions Free radicals that have received some attention in the literature include alkylperoxy radicals, RO_2 OH radicals and singlet oxygen

Overview of TOXI5 Oxidation Reactions

In TOXI5, oxidation is modeled as a general second-order process for the various species and phases of each chemical

$$K_o = [RO_2] \sum_i \sum_j k_{oij}\, f_{ij} \qquad (7\ 75)$$

where

K_o = net oxidation rate constant, day ^{1}

$[RO_2]$ = molar concentration of oxidant, moles/L

k_{oij} = second order oxidation rate constant for chemical as specie i in phase j L/mole-day

The reaction coefficients may be specified as constants, with activation energy constants left as 0 If the user wants TOXI5 to determine rates based on the temperature based Arrhenius function, then non-zero activation energies specified as constants will invoke the following calculation for each rate constant k

$$k(T_K) = k(T_R)\ \exp[1000\ E_{ao}\,(T_K - T_R)/(RT_K\ T_R)] \qquad (7\ 76)$$

where

E_{ao} = Arrhenius activation energy for oxidation reaction, kcal/mole-袁

Activation energies may be specified for each ionic specie simulated If no activation energies are given, then rate constants will not be adjusted to ambient water temperatures

Because of the large number of alkylperoxy radicals that potentially exist in the environment, it would be impossible to obtain estimates of k_{ox} for each species Mill et al (1982) propose estimation of a rate coefficient using t-butyl hydroperoxide as a model oxidizing agent They argue that other alkylperoxides exhibit similar reactivities to within an order of magnitude The second-order rate coefficients are input to TOXI5 as constants

In addition to estimating a rate coefficient an estimate of free radical concentrations must be made to completely define the expression for free radical oxidation Mill et al (1982) report RO_2 concentrations on the order of 10^{9} $\underline{M}$ and OH concentrations on the order of 10^{17} $\underline{M}$ for a limited number of water bodies Zepp et al (1977) report an average value on the order of 10^{12} $\underline{M}$ for singlet oxygen in water bodies sampled The source of free radicals in natural waters is photolysis of naturally occurring organic molecules If a water body is turbid or very deep, free radicals are likely to be generated only near the air-water interface, and consequently, chemical oxidation will be relatively less important In such cases, the concentrations cited above are appropriate in only the near-surface zones of water bodies The molar oxidant concentrations are input to TOXI5 using parameter OXRADG (ISEG)

Implementation

Table 7 16 TOXI5 Oxidation Data

Description	Notation	Range	Units
Oxidation rate constant for specie i phase j	k_{oij}		L/mole-day
Activation energy for oxidation of specie i	E_{aoi}	15-25	kcal/mole 袁
Water temperature	T	4-30	蚓
Concentration of oxidants	$[RO_2]$	$10^{17}-10^{8}$	moles/L

TOXI5 oxidation data specifications are summarized in Table 7 16 The water temperature and concentration of oxidants are input parameters, which may be specified for each model segment The temperature may be time variable as well (input as a time series) If an activation energy is not supplied, no temperature corrections will be performed Input data are described below

Oxidation Rate, L/mole-day-- The user may specify second order oxidation rate constants for each phase (dissolved, DOC-sorbed, and sediment-sorbed) and each ionic specie using constant KOX20 Constant numbers for the neutral molecule are summarized in Table 7 17 $KOX20_{11}$ refers to the dissolved neutral chemical, $KOX20_{21}$ refers to the DOC-sorbed neutral chemical, $KOX20_{31}$ refers to the sediment-sorbed neutral chemical Constant numbers for the ionic species are given in Part B of this

Table 7 17 Oxidation Constants

VARIABLE	C_1	C_2	C_3
TREFO	258	858	1458
$KOX20_{11}$	261	861	1461
$KOX20_{21}$	266	866	1466
$KOX20_{31}$	271	871	1471
EOX_1	276	876	1476

document

Activation Energy, kcal/mole-袁-- The user may specify activation energies for each chemical using constant EOX Constant numbers are summarized in Table 7 17 If EOX is omitted or set to 0, oxidation rates will not be affected by temperature

Reference Temperature,蚓-- The user may specify the reference temperature at which oxidation rates were measured using constant TREFO Constant numbers are summarized in Table 7 17 If a reference temperature is not supplied, then a default of 20 蚓 is assumed

Oxidant Concentration, mole/L-- The user should specify segment variable oxidant concentrations using parameter 13, OXRAD (Group G Record 4, PARAM(I 13)

7 9 BIODEGRADATION

Introduction

Bacterial degradation, sometimes referred to as microbial transformation, biodegradation or biolysis, is the breakdown of a compound by the enzyme systems in bacteria Examples are given in Figure 7 6 Although these transformations can detoxify and mineralize toxins and defuse potential toxins, they can also activate potential toxins

Biodegradation encompasses the broad and complex processes of enzymatic attack by organisms on organic chemicals Bacteria and to a lesser extent fungi, are the mediators of biological degradation in surface water systems Dehalogenation, dealkylation, hydrolysis, oxidation, reduction ring cleavage, and condensation reactions are all known to occur either metabolically or via organisms that are not capable of utilizing the chemical as a substrate for growth

Two general types of biodegradation are recognized--growth metabolism and cometabolism Growth metabolism occurs when the organic compound serves as a food source for the bacteria Adaptation times from 2 to 20 days were suggested in Mills et al 1985 Adaptation may not be required for some chemicals or in chronically exposed environments Adaptation times may be lengthy in environments with a low initial density of degraders (Mills et al , 1985) For cases where biodegradation is limited by the degrader population size, adaptation is faster for high initial microbial populations and slower for low initial populations Following adaptation, biodegradation proceeds at fast first-order rates Cometabolism occurs when the organic compound is not a food source for the bacteria Adaptation is

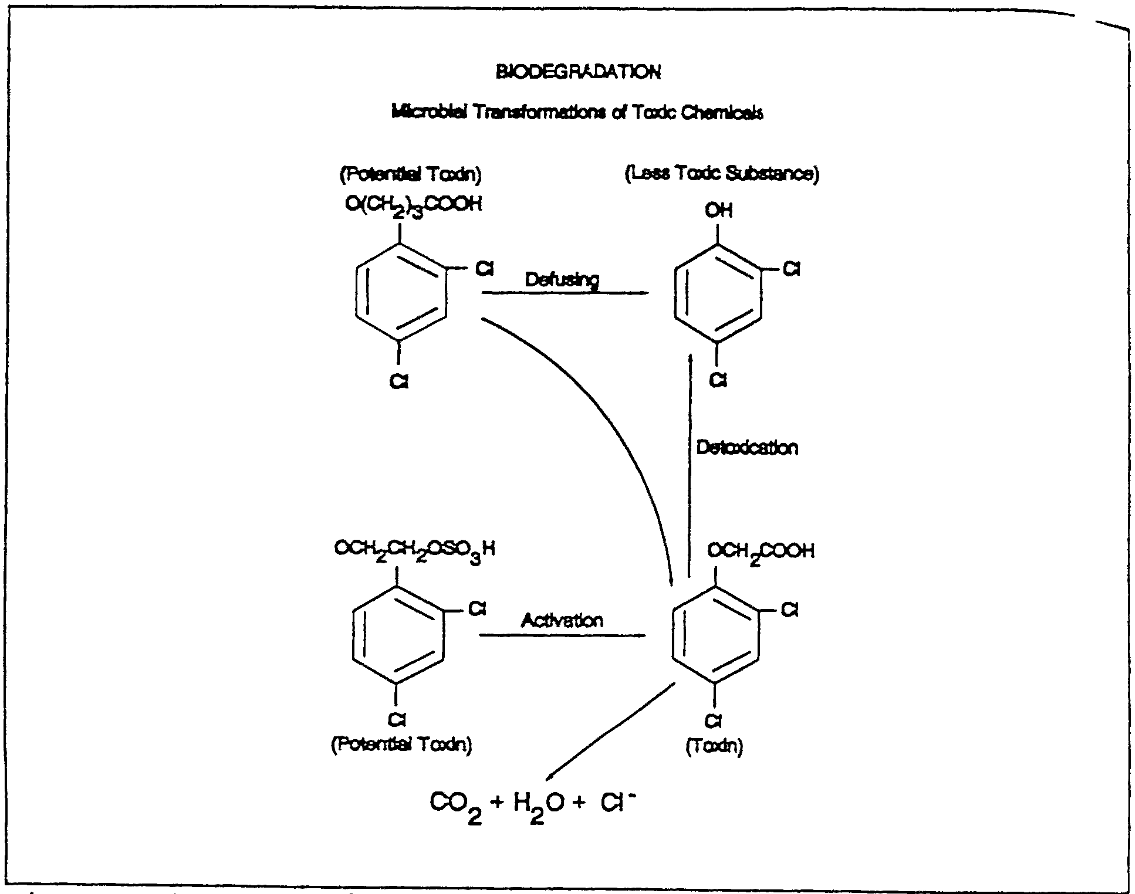


Figure 7 6 Microbial transformations of toxic chemicals (Alexander 1980)

seldom necessary, and the transformation rates are slow compared with growth metabolism

The growth kinetics of the bacterial population degrading a toxic chemical are not well understood The presence of competing substrates and of other bacteria, the toxicity of the chemical to the degrading bacteria and the possibilities of adaptation to the chemical or co-metabolism make quantification of changes in the population difficult As a result, toxic chemical models assume a constant biological activity rather than modeling the bacteria directly Often, measured first order biodegradation rate constants from other aquatic systems are used directly

Overview of TOXI5 Biodegradation Reactions

In TOXI5, first order biodegradation rate constants or half lives for the water column and the benthos may be specified If these rate constants have been measured under similar conditions, this first order approach is likely to be as accurate as more complicated approaches If first order rates are unavailable or if they must be extrapolated to different bacterial conditions, then the second-order approach may be used It is assumed that bacterial populations are unaffected by the presence of the compound at low concentrations Second-order kinetics for dissolved, DOC-sorbed, and sediment-sorbed chemical are considered

$$K_{Bw} = P_{bac}(t) \sum_i \sum_j k_{Bij}\, f_{ij} \qquad j = 1,2 \qquad (7\ 77)$$

$$K_{Bs} = P_{bac}(t) \sum_i \sum_j k_{Bij}\, f_{ij} \qquad j = 3 \qquad (7\ 78)$$

where

K_{Bw} = net biodegradation rate constant in water, day^{1}

K_{Bs} = net biodegradation rate constant on sediment, day^{1}

k_{Bij} = second order biodegradation rate constant for specie i, phase j, ml/cell-day

$P_{bac}(t)$ = active bacterial population density in segment, cell/ml

f_{ij} = fraction of chemical as specie i in phase j

In TOXI5 the biodegradation rate may be adjusted by temperature as shown below

$$k_{Bij}(T) = k_{Bij}\, Q_{Tij}^{(T-20)/10} \qquad (7\ 79)$$

where

Q_{Tij} = 'Q-10 temperature correction factor for biodegradation of specie i phase j

T = ambient temperature in segment, 蚓|

The temperature correction factors represent the increase in the biodegradation rate constants resulting from a 10°C temperature increase Values in the range of 1 5 to 2 are common

Environmental factors other than temperature and population size can limit bacterial rates Potential reduction factors must be considered externally by the user Nutrient limitation can be important in oligotrophic environments

Low concentrations of dissolved oxygen can also cause reductions in biodegradation rates and this effect is not simulated in TOXI5 Below DO concentrations of about 1 mg/L, the rates start to decrease When anoxic conditions prevail, most organic substances are biodegraded more slowly Because biodegradation reactions are generally more difficult to predict than physical and chemical reactions, site-specific calibration becomes more important

Biodegradation can be implemented using segment variable first order rate constants rather than bacterial populations If first order rate constants are input for P_{bac}, then second order rate constants k_{Bij} should be set to 1 0 in equations 7 71 and 7 72

Implementation

TOXI5 biodegradation data specifications are summarized in Table 7 18 The second order rate constants for water and for bed segments can be specified as constants Temperature correction factors can be left at 0 If the user wants TOXI5 to correct the rate constants for ambient segment temperatures, then nonzero temperature correction factors should specified as constants User input for implementing biodegradation is given below

First Order Rates, day^{-1}-- The user may specify first order biodegradation rate constants for water column and benthic segments using constants KBW and KBS If nonzero values are specified for these constants they will be used directly bypassing second order calculations Constant numbers are given in Table 7 19

Second Order Rate Coefficients, mL/cell-day-- The user may specify second order biodegradation rate constants for each phase (dissolved, DOC-sorbed, and sediment-sorbed) and each ionic specie using constant KBIO20 Constant numbers for the neutral molecule are summarized in Table 7 19 KBIO20$_{11}$ refers to the dissolved neutral chemical, KBIO20$_{21}$ refers to the DOC-sorbed neutral chemical, KBIO20$_{31}$ refers to the sediment-sorbed neutral chemical Constant numbers for the ionic species are given in Part B of this document

Table 7 18 TOXI5 Bacterial Degradation Data

Description	Notation	Common Range	Units
Observed first order degradation rate in water column	K_{Bw}	0-0 5	day ^{1}
Observed first order degradation rate in benthos	K_{Bs}	0-0 5	day^{-1}
Bacterial activity or concentration of bacterial agent	P_{bac}	10^2-10^7	cells/mL
Observed second-order rate coefficients for specie i	k_{Bij}	0-10 ^{6}	mL/cell-day
Biodegradation temperature coefficients for specie i phase j	Q_{Tij}	1 5-2 5	-
Water temperature	T	4-30	°C

Temperature Coefficients-- The user may specify temperature correction factors for the dissolved, DOC-sorbed, and sediment-sorbed phase of each chemical using constants Q10DIS, Q102DOC, and Q10PAR respectively These constants represent the multiplication factor for biodegradation rates corresponding to a 10 °C temperature increase Constant numbers are summarized in Table 7 19 If Q10 values are omitted or set to 0 biodegradation rates will not be affected by temperature

Table 7 19 Biodegradation Constants

VARIABLE	C_1	C_2	C_3
KBW	141	741	1341
KBS	142	742	1342
KBIO2O$_{11}$	146	746	1346
KBIO20$_{21}$	151	751	1351
KBIO20$_{31}$	156	756	1356
Q10DIS$_1$	161	761	1361
Q10DOC$_1$	166	766	1366
Q10PAR$_1$	171	771	1371

Bacterial Population Levels, cell/mL-- The user may specify segment and time variable bacterial concentrations using parameter 14, BAC and time funcions 16 and 17, BACNW and BACNS Typical population size ranges are given in Table 7 19
If bacterial concentrations are to remain constant in time, the user should enter segment mean concentrations using parameter BAC BACNW and BACNS should be omitted

Table 7 20 Size of Typical Bacterial Populations in Natural Waters

Water Body Type	Bacterial Numbers (cells/ml)	Ref
Oligotrophic Lake	50 - 300	a
Mesotrophic Lake	450 - 1,400	a
Eurtophic Lake	2000 - 12,000	a
Eutrophic Reservoir	1000 - 58,000	a
Dystrophic Lake	400 - 2,300	a
Lake Surficial Sediments	$8x10^9$ - $5x10^{10}$ cells/100 g dry wt	a
40 Surface Waters	500 - $1x10^6$	b
Stream Sediments	10^7 - 10^8 cells/100 g	c
Rur River (winter)	$3x10^4$	d

References

[a]Wetzel (1975) Enumeration techniques unclear

[b]Paris *et al* Bacterial enumeration using plate counts

[c]Herbes & Schwall (1978) Bacterial enumeration using plate counts

[d]Larson *et al* (1978) Bacterial enumeration using plate counts

The user may enter time-variable water column and benthic bacterial concentrations via time functions BACNW and BACNS respectively as a series of concentration versus time values Parameter BAC will then represent the ratio of each segment concentration to the time function values The product of BAC and the BACNW or BACNS function gives the segment and time specific bacterial concentrations used by TOXI5 (Group G, Record 4, PARAM(I,14) Group I, Record 2 VALT(16,K) VALT(17,K),

7 10 EXTRA REACTION

Introduction

An extra second-order reaction is included in TOXI5 The second order reaction allows the user to simulate the effect of processes not considered by TOXI5 The reaction depends upon a rate constant and a enviromnetal paramater which may be taken to represent, for example, some reducing or oxidizing agent The rate of reaction may also vary with temperature

Overview of TOXI5 Extra Reaction

TOXI5 allows the user to specify an additional second order reaction for the various species and phases of each chemical

$$K_E = [E] \sum_i \sum_j k_{eij} \, f_{ij} \qquad (7\ 80)$$

where

K_E = net extra reaction rate constant, day^{1}

[E] = intensity of environmental property driving this reaction

k_{eij} = second order rate constant for chemical as specie in phase j, in [E]^{1} day^{1}

f_{ij} = fraction of chemical as specie i in phase j

The reaction coefficients may be specified as constants with activation energy constants left as 0 If the user wants TOXI5 to determine rates based on the temperature based Arrhenius function, then non-zero activation energies specified as constants will invoke the following calculation for each rate constant k

$$k_e(T_K) = k_e(T_R) \exp[1000 \, E_{ae}(T_K - T_R)/(RT_K \, T_R)] \qquad (7\ 81)$$

where

E_{ae} = Arrhenius activation energy for extra reaction kcal/mole-衰

Activation energies may be specified for each ionic specie simulated If no activation energies are given then rate constants will not be adjusted to ambient water temperatures

An example of a kinetic process that may be modeled as this extra reaction is reduction If reduction is modeled, [E] may be interpreted as the concentration of environmental reducing agents

RH_2, so that

$$C + RH_2 \rightarrow P \tag{7 82}$$

and

[E] = concentration of RH_2, moles/L

k_e = second order rate constant, L/mole-day

P = reduced product

The identity of the reducing agent and the second order rate constant must be identified and quantified by laboratory kinetics studies If both the environmental oxidizing and reducing agents are in excess, then two chemicals may be simulated as a redox pair

$$C_1 + RO_2 \rightleftharpoons C_2 + RH_2 \tag{7 83}$$

where

C_1 = reduced chemical

C_2 = oxidized chemical

RO_2 = oxidizing agent

PH_2 = reducing agent

Laboratory kinetics studies can control the concentrations of RO_2 and RH_ to determine rate constants for both oxidation and reduction These may be specified as constants k_{ox} and k_E Yield coefficients Y_{012} and Y_{021} must also be specified as constants The spatially variable concentrations $[RO_2]$ and $[RH_2]$ must be specified as parameters

Implementation

The input data requirements for the second order reactions include the second order reaction rate constants which may be specified for each specie and sorbed form (dissolved DOC sorbed and sorbed to particulate) If the rates are to be temperature corrected, then the user may supply the reference temperature at which the extra reaction rates were measured and the activation energy for the reaction The rates will then be adjusted using a temperature-based Arrhenius function If an activation energy is not supplied no temperature corrections will be performed The extra property of the aquatic environment that affects the extra reaction is specified to the model as a parameter which may vary between segments The units of the 'extra' property must be consistent with those used for the second-order rate constant The product of the extra property and second-order rate constant must have units of day^{1} The temperature may be time variable as well (input as a time series) Input data are described below

Extra Reaction Rate, L/mole-day-- The user may specify second order extra rate constants for each phase (dissolved DOC-sorbed, and sediment-sorbed) and each ionic specie using constant KE20 Constant numbers for the neutral molecule are summarized in Table 7 21 KE20$_{11}$ refers to the dissolved neutral chemical, KE20$_{21}$ refers to the DOC-sorbed neutral chemical, KE20$_{31}$ refers to the sediment-sorbed neutral chemical Constant numbers for the ionic species are given in Part B of this document

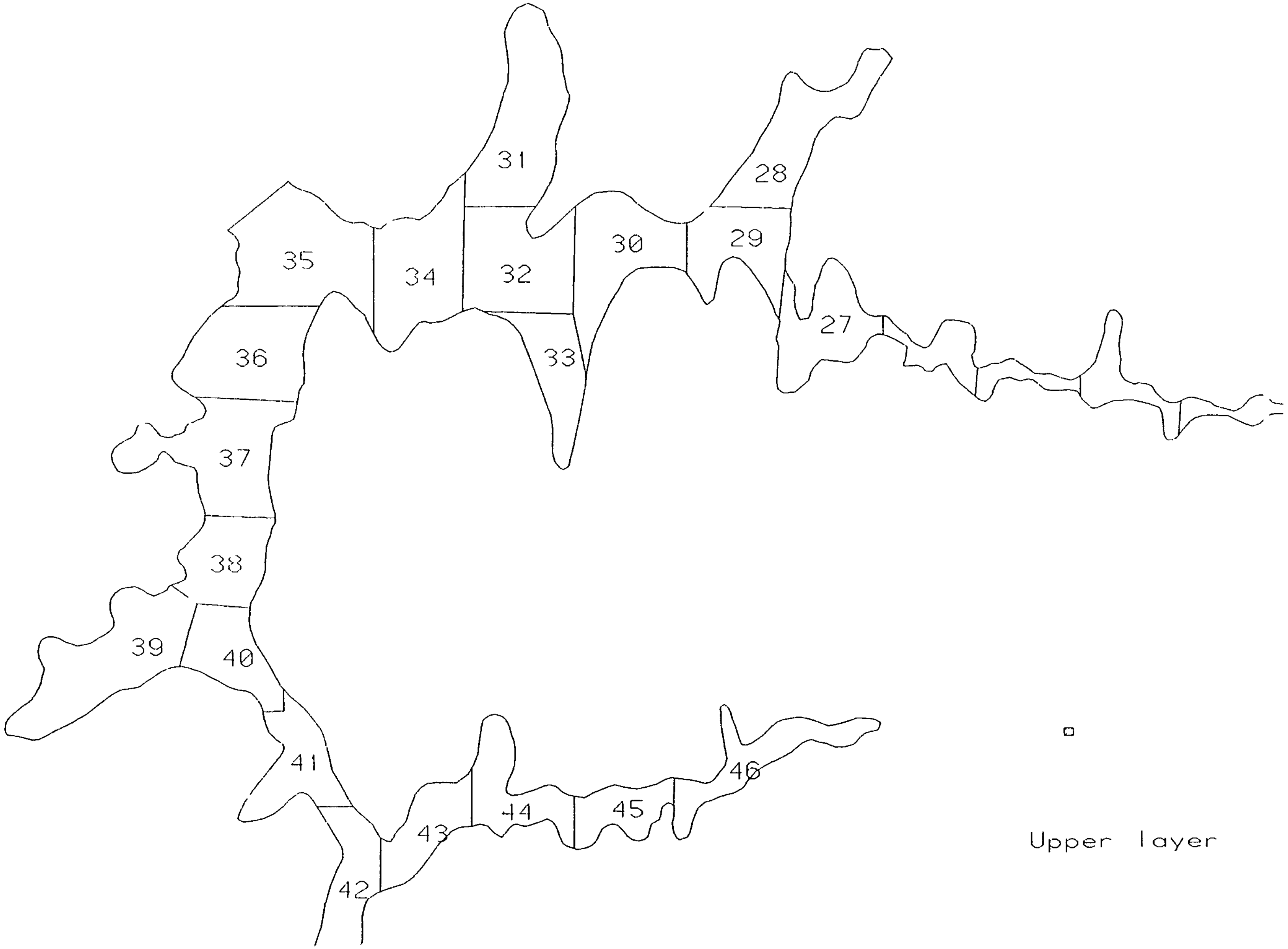
Table 7 21 Extra Reaction Constants

VARIABLE	C_1	C_2	C_3
TREFE	573	1173	1773
KE20$_1$	576	1176	1776
KE20$_{21}$	581	1181	1781
KE20$_{31}$	586	1186	1786
EEX$_1$	591	1191	1791

Activation Energy, kcal/mole-°K-- The user may specify activation energies for each chemical using constant EEX Constant numbers are summarized in Table 7 21 If EEX is omitted or set to 0, oxidation rates will not be affected by temperature

Reference Temperature, °C-- The user may specify the reference temperature at which oxidation rates were measured using constant TREFE Constant numbers are summarized in Table 7 21 If a reference temperature is not supplied then a default of 20 °C is assumed

Extra Environmental Concentration, mole/L-- The user should specify segment variable extra environmental concentrations using parameter 15 EXENV (Group G, Record 4, PARAM(I,15)



Upper layer

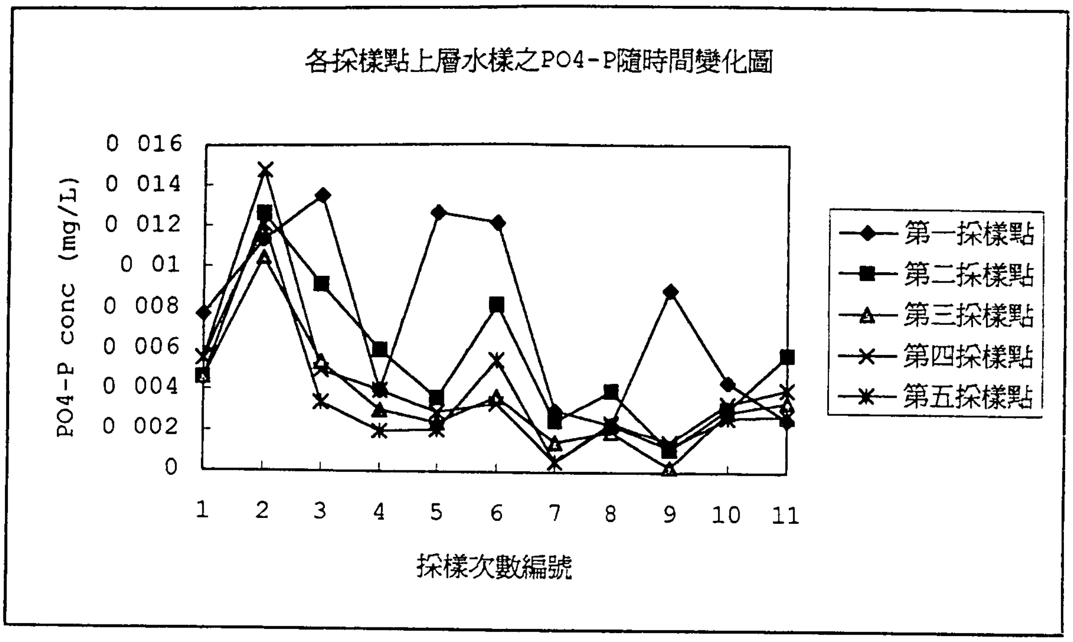


圖 4 2 各採樣點上層水樣之PO4-P隨時間變化圖

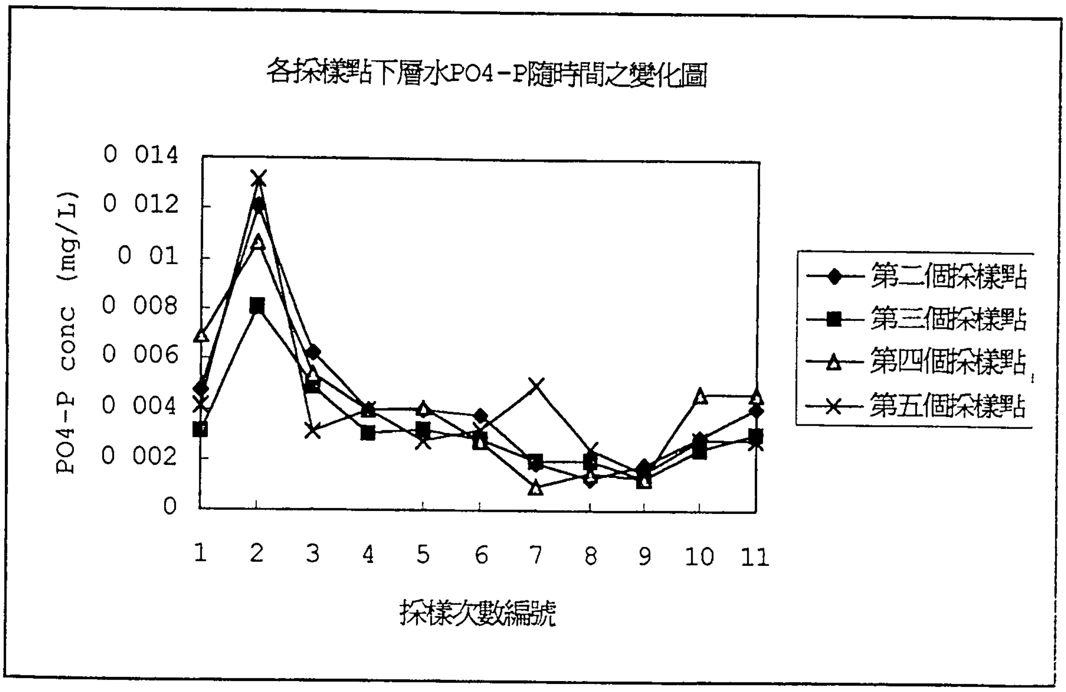


圖 4 3 各採樣點下層水PO4-P隨時間之變化圖

THE WATER QUALITY ANALYSIS SIMULATION PROGRAM, WASP5

PART B:

THE WASP5 INPUT DATASET

Version 5 00, May 31, 1993

by

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CONTENTS

CHAPTER 1

INTRODUCTION

RESTART OUT

* INP (input file)

* MSB

* TRN

* OUT

* EDF * TDF

* RST

See P 77 for description

We got RESTART. -ust ???

1 1 GENERAL CONSIDERATIONS

This section describes the input required to run the WASP5 water quality program The user should be cautioned about potential changes to the dataset or manual that may accompany version updates of the software The printed manual may become dated as enhancements are made or errors are identified and corrected Please download the latest manual accompanying the current version of WASP5

To arrange the input into a logical format, WASP5 data are divided into 10 groups, A through J

A - Model Identification and Simulation Control

B - Exchange Coefficients

C - Volumes

D - Flows

E - Boundary Concentrations

F - Waste Loads

G - Environmental Parameters

H - Chemical Constants

I - Time Functions

J - Initial Conditions

The following is a brief explanation of each data group

DATA GROUP A provides for descriptive model identification and contains simulation control options The user must specify the number of segments and the number of systems The user must also specify calculational time steps and print intervals here

DATA GROUP B contains dispersive exchange information Dispersion occurs between segments and along a characteristic length Dispersion coefficients vary with time in a piecewise linear time function

DATA GROUP C supplies initial segment volume information and information on the segment type and underlying segment numbers Hydraulic geometry information can be given to derive segment average depth and velocity as a function of flow These values are used in reaeration and volatilization calculations only (not in the basic transport calculations)

DATA GROUP D supplies flow and sediment transport information between segments Flows may be contained in the WASP input dataset, or may be imported from an external hydrodynamic file Flows in the WASP5 input dataset vary with time following a piecewise linear time function

DATA GROUP E supplies concentrations for each system at the boundaries All system concentrations must be supplied for each boundary Boundary concentrations vary with time in a piecewise linear time function

DATA GROUP F defines the waste loads and segments that receive the waste loads for both point and diffuse sources Point source loads vary with time in a piecewise linear time fuction Nonpoint source loads vary with time in a daily step function

DATA GROUP G contains appropriate environmental characteristics of the water body These parameters are spatially variable, varying with each model segment

DATA GROUP H contains appropriate chemical characteristics or constants Constants in WASP remain constant in both time and space

DATA GROUP I contains appropriate environmental or kinetic time functions

DATA GROUP J contains initial concentrations for each segment and each system along with dissolved fractions and the density of solids systems

The input dataset is a formatted ASCII file The user must carefully place input data in the appropriate fields, and be sure to right justify integers

1 2 THE EUTROPHICATION MODEL

EUTRO4 requires the same input format as the basic WASP5 model This format is explained in detail in the chapters below This section summarizes the variables needed specifically for EUTRO4

As described in detail in Chapter 5, the 8 systems for eutrophication modeling are ammonia nitrogen nitrate nitrogen, inorganic phosphorus, phytoplankton carbon, carbonaceous BOD,

Table 1 EUTRO4 Systems and Levels of Complexity

System Number	Symbol	Name	Use in Complexity Level 1	2	3	4	5	6
1	NH3	Ammonia nitrogen		X	X	X	X	X
2	NO3	Nitrate nitrogen			X	X	X	X
3	PO4	Inorganic phosphorus				X	X	X
4	CHL	Phytoplankton carbon				X	X	X
5	CBOD	Carbonaceous BOD	X	X	X	X	X	X
6	DO	Dissolved oxygen	X	X	X	X	X	X
7	ON	Organic nitrogen			X	X	X	X
8	OP	Organic phosphorus				X	X	X

Complexity Level	Explanation
1	"Streeter-Phelps BOD-DO with SOD
2	"Modified Streeter-Phelps with NBOD
3	Linear DO balance with nitrification
4	Simple eutrophication
5	Intermediate eutrophication
⑥	Intermediate eutrophication with benthos

dissolved oxygen, organic nitrogen and organic phosphorus Table 1 summarizes these systems and their use in six discrete levels of complexity

The user should note that these discrete levels of complexity are suggestive only The user may choose to simulate any combination of these variables using any combination of the parameter functions and values described below In fact, during calibration, the user may choose to simulate only one variable such as CBOD, while bypassing (and thus holding constant) all other variables

1 3 THE TOXIC CHEMICAL MODEL

TOXI4 requires the same input format as the basic WASP5 model This format is explained in detail in the chapters below This section summarizes the variables needed specifically for TOXI4

Table 2 TOXI4 Systems and Levels of Complexity

System Number	Symbol	Name	Levels of Complexity for Solids 1, 2	3	4	Kinetics 1-3	4
1	C_1	Chemical 1	x	x	x	x	x
2	S_1	Solid 1		x	x		
3	S_2	Solid 2			x		
4	S_3	Solid 3			x		
5	C_2	Chemical 2					x
6	C_3	Chemical 3					x

Complexity Level	Explanation
Solids 1	Descriptive Solids concentration field
Solids 2	Descriptive solids concentration field with specific solids transport rates
Solids 3	Simulated total solids
Solids 4	Three simulated solids types
Equil 1	Constant partition coefficient
Equil 2	Spatially-variable partition coefficients
Equil 3	Hydrophobic sorption
Equil 4	Solids-dependent partitioning
Equil 5	Sorption plus ionic speciation
Kinetic 1	Constant half lives or rate constants
Kinetic 2	Spatially-variable rate constants
Kinetic 3	Second order rates
Kinetic 4	Transformation products

As described in Chapter 7 the 6 systems for toxicant modeling are chemical 1, solids fraction 1, solids fraction 2, solids fraction 3 chemical 2 and chemical 3 Table 2 summarizes these systems and their use in several discrete levels of complexity These levels of complexity describe possible approaches to simulating solids, equilibrium reactions, and kinetic reactions They are suggestive only The user may choose to simulate any combination of these variables using any combination of the parameter functions and values described below

CHAPTER 2

DATA GROUP A MODEL IDENTIFICATION AND SIMULATION CONTROL

Basic simulation information is provided in Data Group A beginning with titles and descriptions in Records 1 and 2. The number of systems (state variables) and segments are specified in Record 4. Calculational time steps are provided in Records 6 and 7, and print intervals in Records 8 and 9. System bypass options are set in Record 10.

2.1 RECORD FORMATS

Record 1--Title of Simulation (A5, A75)

SIMTYP = type of simulation, TOXI4 = toxics dataset EUTRO = eutrophication dataset (A5)

TITLE1 = descriptive title of simulation (A75)

actually, both are read [illegible] only see [illegible] 159/160

Record 2--Description of Simulation (A80)

TITLE2 = description of simulation (A80)

Record 3--Record 4 Names (A80)

HEADER = names of Record 4 variables, positioned properly, for user convenience only (A80)

Record 4--Simulation Control Parameters (7I5, 2F5.0, F3.0, F2.0)

NOSEG = number of segments in model network (I5)

NOSYS = number of model systems (state variables) (I5) (See Table 1) [illegible]

ICFL = flag controlling use of restart file 0 = neither read from nor write to restart file (initial conditions located in input file), 1 = write final simulation results to restart file (initial conditions located in input file) 2 = read initial conditions from restart file created by earlier simulation and write final simulation results to new restart file (I5)

0 不用RESTART [illegible]
1 int al cond from ~~input file~~/write final to
2. Read int al from and write final to

MFLAG = flag controlling messages printed on screen during simulation, 0 = all messages printed 1 = simulation time only printed 2 = all messages are suppressed (I5)

~~(IDMP)~~
JMASS = system number for which mass balance analysis will be performed, 0 = no mass balance table generated (I5) will not have MSB file

NEGSLN = negative solution option 0 = prevents negative solutions, ① = allows negative solutions (I5) for first trial

INTYP = time step option 0 = user inputs time step history, 1 = model calculates time step (I5)

ADFAC = advection factor, 0 = backward difference, 0 5 = central difference, 0-0 4 recommended (F5 0)

$f_1 + f_2$ Conc2 + (Conc +ADV

velocity f(time t) → q hydro f((t 4))

ZDAY = day at beginning of simulation 1 is first day (F5 0)

ZHR = hour at the beginning of simulation (F3 0)

ZMIN = minute at the beginning of simulation (F2 0)

TFLG = switch controlling generation of transport file, 0 = generate file, 1 = do not generate file (I5) net TRN

Record 5--Runtime Print Segments (6I5)

ISEGOUT = up to six segment numbers to display at runtime if there are six or more segments in the model network, the user should specify six print segment numbers (I5)

Record 6--Number of Time Steps (I5)

NOBRK = number of different model time steps (I5)

Record 7--Time Steps (4(F10 0, F10 0))

DTS(I) = time step to be used until time T(I), days (F10 0)

T(I) = time up to when time step DTS(I) will be used, days (F10 0)

Record 8--Number of Print Intervals (I5)

NPRINT = number of print intervals (I5)

Record 9--Print Intervals (4(F10 0, F10 0))

PRINT(I) = print interval to be used until time TPRINT(I), days (F10 0)

TPRINT(I) = time up to when print interval PRINT(I) will be used, days (F10 0)

Record 10--System Bypass Options (16I5)

SYSBY(K) = bypass option for system K, 0 = system will be simulated, 1 = system will be bypassed (I5)

2 2 THE EUTROPHICATION MODEL

When running EUTRO4, the number of systems, NOSYS, must be set to 8 in Record 4 The bypass options in Record 10 SYSBY(K) should be set to 0 for those variables checked in the relevant complexity level in Table 1 they should be set to 1 for those variables not checked in the relevant complexity level in Table 1

2 3 THE TOXIC CHEMICAL MODEL

When running TOXI4, the number of systems, NOSYS, can be set from 1 to 6 in Record 4, depending upon the solids and kinetic complexity levels chosen for simulation The bypass options in Record 10 SYSBY(K), should be set to 0 for those variables checked in the relevant complexity level in Table 2 they should be set to 1 for those variables not checked in the relevant complexity level in Table 2

CHAPTER 3

DATA GROUP B EXCHANGE COEFFICIENTS

Exchange coefficients for surface water and pore water are computed from input dispersion coefficients, cross-sectional areas, and characteristic lengths. Dispersion coefficients may vary in time according to piecewise-linear time functions, with groups of segment pairs having the same dispersion time function. Exchange data are read for each exchange field. Field one contains dispersion coefficients for water column exchanges. Field two contains exchange data for pore water exchange.

3.1 RECORD FORMATS

Record 1--Number of Exchange Fields (I5, 75X)

NRFLD = number of exchange fields. NRFLD will generally equal 2 for water column and pore water exchanges. (I5)

TITLE = name of data group. (75X)

If no exchange rates are to be read, set NRFLD to zero and continue with Data Group C. If only surface water exchanges are to be read, set NRFLD to 1 and input the proper values in records 2-6 and 12. If pore water exchanges are to be read, set NRFLD to 2 and input the proper values in records 2-12.

Record 2--Exchange Time Functions for Surface Water Field (I5, 2F10.0)

NTEX(1) = number of exchange time functions for field 1. (I5)

SCALR = scale factor for exchange coefficients. All exchange coefficients for field 1 will be multiplied by this factor. (F10.0)

CONVP = conversion factor for exchanges in field 1. (F10.0)

To skip surface water exchange field, set NTEX(1) to zero and continue with the pore water exchange field (record 7) or the exchange bypass options (record 12).

Records 3-6 are input as a group NTEX(1) times.

Record 3--Exchange Data (I5)

NORS(1,NT) = number of exchanges for field 1, time function NT (I5)

Record 4--Areas, Characteristic Lengths (2F10.0, 2I5)

A(K) = area in square meters for exchange pair K (F10.0)

EL(K) = characteristic length in meters for exchange pair K (F10.0)

IR(K),JR(K) = segments between which exchange occurs. The order of the segments is unimportant (2I5)

Record 4 is repeated NORS(1,NT) times

Record 5--Number of Breaks in Time Function (I5)

NBRKR(1,NT) = number of values and times used to describe dispersion coefficient piecewise-linear time function (I5)

Record 6--Piecewise Linear Dispersion Time Function (4(F10.0, F10.0))

RT(K) = value of dispersion coefficient in m^2/sec at time TR(K) (F10.0)

TR(K) = time in days (F10.0)

Record 6 is repeated NBRKR(1 NT)/4 times

Record 7--Exchange Time Functions for Pore Water Field (I5, 2F10.0)

NTEX(2) = number of exchange time functions for field 2 (I5)

SCALR = scale factor for exchange coefficients. All exchange coefficients for field 2 will be multiplied by this factor (F10.0)

CONVR = conversion factor for exchanges in field 2 (F10.0)

To skip pore water exchange field, set NTEX(2) to zero and continue with record 12

Nt, NRFLD = 1 is enough to skip

Records 8-11 are input as a group NTEX(2) times

Record 8--Exchange Data (I5)

NORS(2,NT) = number of exchanges for field 2, time function NT (I5)

NT = 1, NTEX(2)

Record 9--Areas, Characteristic Lengths (2F10.0, 2I5)

A(K) = area in square meters for exchange pair K (F10.0)

EL(K) = characteristic length in meters for exchange pair K (F10.0)

IR(K),JR(K) = segments between which exchange occurs. The order of the segments is unimportant (2I5)

Record 9 is repeated NORS(2,NT) times

Record 10--Number of Breaks in Time Function (I5)

NBRKR(2,NT) = number of values and times used to describe dispersion coefficient piecewise-linear time function (I5)

Record 11--Piecewise Linear Dispersion Time Function (4(F10.0, F10.0))

RT(K) = value of dispersion coefficient in m^2/sec at time TR(K) (F10.0)

TR(K) = time in days (F10.0)

Record 11 is repeated NBRKR(2,NT)/4 times

Record 12--Exchange Bypass Options (16I5)

RBY(K) = exchange bypass option for system K. 0 = exchange occurs in system K. 1 = bypass exchange for system K (I5)

K = 1, NOSYS

Record 1 is entered once for Data Group B. Records 2 through 6 are input for the surface-water exchange field with Records 3, 4, 5, and 6 being repeated for each time function in this exchange field Record 4 uses as many lines as necessary to input NORS sets of A(K), EL(K), IR(K), and JP(K), with 1 set on each line Record 6 uses as many lines as needed to input NBRKP pairs of RT(K) and TR(K), with 4 pairs occupying each line

Records 7 through 11 are input for the pore water exchange field, with Records 8 9, 10, and 11 being repeated for each time function in this exchange field Record 9 uses as many lines as necessary to input NORS sets of A(K), EL(K), IR(K), and JR(K) with 1 set on each line Record 11 uses as many lines as needed to input NBRKR pairs of RT(K) and TR(K), with 4 pairs occupying each line

After data for all exchange fields are entered, Record 12 is input on the following line with NOSYS entries

CHAPTER 4

DATA GROUP C   VOLUMES

Initial segment volumes are provided in Data Group C   In addition, segment type and underlying segment numbers are specified   Hydraulic geometry information can be given to derive segment average depth and velocity as a function of flow   These values are used in reaeration and volatilization calculations only (not in the basic transport calculations)

4 1   RECORD FORMATS

Record 1--Preliminary Data (2I5, F10.0, 60X)

IVOPT = water column volume option -- 1 = constant water column volumes, 2 3 = volumes adjusted to maintain flow continuity (I5)

IBEDV = benthic volume option -- 0 = constant bed volumes, 1, bed volumes change in response to sediment transport (I5)

TDINTS = benthic time step in days for recomputing porosity (if IBEDV = 0) or for sediment bed compaction (if IBEDV = 1) (F10 0)

TITLE = name of data group (60X)

Record 2--Scale Factors (2F10.0)

SCALV = scale factor for volumes   All volumes will be multiplied by this factor (F10 0)

CONVV = conversion factor for volumes   (F10 0)

Record 3 is repeated NOSEG times

Record 3--Segment Types and Volumes (3I10, 5F10.0)

ISEG = segment number

IBOTSG = segment immediately below ISEG (I10)

ITYPE(ISEG) = segment types 1 = surface water segment 2 = subsurface water segment, 3 = upper bed segment, 4 = lower bed segment   (I10)

BVOL(ISEG) = volume of segment ISEG in cubic meters

(F10 0)

VMULT(ISEG) = hydraulic coefficient "a' for velocity in ISEG as a function of flow

$$v = a\,Q^b$$

If b = 0, VMULT is a constant velocity in m/sec (F10 0)

VEXP(ISEG) = hydraulic exponent "b" for velocity in ISEG as a function of flow (0-1) A value of 0 4 represents rectangular channels (F10 0)

DMULT(ISEG) = hydraulic coefficient c" for depth of ISEG as a function of flow

$$d = c\,Q^d$$

If d = 0, DMULT is a constant depth in m (F10 0)

DXP(ISEG) = hydraulic exponent d for depth of ISEG as a function of flow (0-1) A value of 0 6 represents rectangular channels (F10 0)

Note that the four hydraulic geometry parameters are used to calculate segment velocity and depth, which are not used by WASP5 in transport calculations These are used to calculate reaeration or volatilization from segments

Records 1 and 2 are entered once for Data Group C Record 3 is repeated NOSEG times If ICFL = 2 in Data Group A, volumes are read from the restart file (* RST where * is the input data set name) and Records 2 and 3 should not be included in the input data set

CHAPTER 5

DATA GROUP D FLOWS

5 1 RECORD FORMATS

Data Group D provides for the advective transport flows that are used in the model Flows may be input for up to 6 transport fields Field one consists of advective flows in the water column Field two consists of pore water flows Fields three, four, and five consist of sediment transport velocities and cross-sectional areas for solids A separate sediment transport field is specified for each of up to 3 solids types Field six is for evaporation and precipitation velocities and cross-sectional areas All flows may vary in time according to piecewise linear time functions for To

Record 1 is read first If IQOPT = 1 or 2, Data Block D1 is read next, if IQOPT = 3, Data Block D1 is skipped Data Blocks D2, D3, D4, D5 and D6 follow in order for NFIELD = 2, 3, 4, 5, and 6, respectively Following all specified Data Blocks, Record 32 is read

Record 1--Data Input Options, Number of Flow Fields (2I5, A12)

IQOPT = flow option

1 = field one (advective) flows are specified directly by user Individual flows at each segment interface are summed by the model and the net flow is applied across the interface

2 = field one flows are specified directly by the user Individual flows at each segment interface are applied directly by the model

3 = flows are read from a formatted file created by DYNHYD5 or other hydrodynamic model (I5)

NFIELD = number of flow fields The first two fields are surface water and pore water flows An additional field (3 4 or 5) is used for each type of solid modeled Field 6 is used for evaporation and precipitation If no flows are used, set NFIELD to zero and continue with Data Group E (I5)

HYDFIL = name of hydrodynamic file to be read by WASP5 during the simulation (for example, RIVER1 HYD) (A12)

only used for ICOPT = 3? check of/o

DATA BLOCK D1 Direct Input of Field One Flows (IQOPT = 1,2)

Record 2--Number of Flow Time Functions (I5, 2F10.0)

NINQ(1) = number of time functions for Field One If no flows are used in field one, set NINQ to zero and skip to next field (I5)

SCALQ = scaling factor All flows in Field one are multiplied by SCALQ (F10 0)

CONVQ = units conversion factor (F10 0)

Records 3 - 6 are input as a group NINQ(1) times

Record 3--Number of Flows (I5)

NOQS(1,NI) = number of unit flow responses in field one time function NI each unit flow is defined for a single segment pair (I5)

Record 4--Flow Routing for Field One (4(F10 0, 2I15))

BQ(1,NI,K) = portion of flow for field one, time function NI that flows between segment pair K (F10 0)

JQ(1,NI,K) = upstream segment (I5)

IQ(1,NI,K) = downstream segment (I5)

Record 4 is repeated NOQS(1,NI)/4 times

Record 5--Number of Breaks in Advective Time Functions (I5)

NBRKQ(1,NI) = the number of flows and times used to describe piecewise linear time function NI (I5)

Record 6--Piecewise Linear Advective Time Function (4(2F10.0))

/ QT(1,NI,K) = advective flow in m^3/s (F10 0)

TQ(1,NI K) = time in days (F10 0)

Record 6 is repeated NBRKQ(1,NI) times

Record 2 is input once for Data Block D1. Records 3, 4, 5, and 6 are input once for each flow time function. Record 4 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets per line. Record 6 uses as many lines as necessary to input NBRKQ sets of QT and TQ with four sets on each line.

DATA BLOCK D2 Field Two (Pore Water) Flows

Record 7--Number of Pore Water Time Functions (I5, 2F10.0)

NINQ(2) = number of pore water time functions. If no flows are used in Field Two, set NINQ to zero and skip to sediment transport fields. (I5)

SCALQ = scaling factor for pore water flows (F10.0)

CONVQ = units conversion factor (F10.0)

Records 8 - 11 are input as a group NINQ(2) times

Record 8--Number of Flows (I5)

NOQS(2,NI) = number of segment pair flows in Field 2, time function NI (I5)

Record 9--Flow Routing for Field Two (4(F10.0, 2I5))

BQ(2,NI,K) = portion of pore water flow for time function NI that flows between segment pair K (F10.0)

JQ(2,NI,K) = upstream segment (I5)

IQ(2,NI,K) = downstream segment (I5)

Record 9 is repeated NOQS(2,NI)/4 times

Record 10--Number of Breaks in Pore Water Time Function (I5)

NBRKQ(2,NI) = number of pore water flows and times used to describe piecewise linear time function NI (I5)

Record 11--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(2,NI,K) = pore water flow in m^3/s (F10.0)

TQ(2,NI,K) = time in days (F10.0)

Record 11 is repeated NBRKQ(2,NI)/4 times

Record 7 is input once for Data Group D2. Records 8, 9, 10 and 11 are input once for each pore water time function. Record 9 uses as many lines as necessary to input NOQS sets of BQ, JQ and IQ, with four sets on each line. Record 11 uses as many lines as necessary to input NBRKQ sets of QT and TQ, with four sets on each line.

DATA BLOCK D3 Sediment 1 Transport Field

Sediment transport flow data are input as velocities and areas. Velocities may vary in time and represent settling, sedimentation, deposition, and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids are modeled, skip directly to Record 32 (Flow Bypass Options).

Record 12--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(3) = number of velocity time functions for Field 3 (I5)

SCALQ = scaling factor for velocities (F10.0)

CONVQ = units conversion factor (F10.0)

Records 13 - 16 are input as a group NINQ(3) times

Record 13--Number of Segment Pairs (I5)

NOQS(3,NI) = number of segment pairs involved in sediment 1 transport (I5)

Record 14--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(3,NI,K) = area in square meters between segment pair K (F10.0)

JQ(3,NI,K) = segment sediment is transported from (I5)

IQ(3,NI,K) = segment sediment is transported to (I5)

Record 14 is repeated NOQS(3,NI)/4 times

Record 15--Number of Breaks in Velocity Time Function (I5)

NBRKQ(3,NI) = number of velocities and times used to describe piecewise linear time function NI (I5)

Record 16--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(3,NI,K) = sediment 1 transport velocity in m/s (F10 0)

TQ(3,NI,K) = time in days (F10 0)

Record 16 is repeated NBRKQ(3,NI)/4 times

Record 12 is input once for Data Block D3   Records 13, 14, 15 and 16 are input for each velocity time function   Record 14 uses as many lines as needed to input NOQS sets of BQ, JQ and IQ with four sets on one line   Record 16 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line

DATA BLOCK D4   Sediment 2 Transport Field

Sediment transport flow data are input as velocities and areas   Velocities may vary in time, and represent settling sedimentation, deposition, and scour   Only solids and sorbed chemical are transported by these fields   A separate field is specified for each sediment size fraction   If no solids 2 are modeled, enter 0 for NINQ(4) then skip directly to the next data block

Record 17--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(4) = number of velocity time functions for Field 4 (I5)

SCALQ = scaling factor for velocities (F10 0)

CONVQ = units conversion factor (F10 0)

Records 18 - 21 are input as a group NINQ(4) times

Record 18--Number of Segment Pairs (I5)

NOQS(4 NI) = number of segment pairs involved in sediment 2 transport (I5)

Record 19--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(4,NI,K) = area in square meters between segment pair (F10.0)

JQ(4,NI,K) = segment sediment is transported from (I5)

IQ(4,NI,K) = segment sediment is transported to (I5)

Record 19 is repeated NOQS(4,NI)/4 times

Record 20--Number of Breaks in Velocity Time Function (I5)

NBRKQ(4,NI) = number of velocities and times used to describe piecewise linear time function NI (I5)

Record 21--Piecewise Linear Velocity Time Function (4(2F10.0))

/ QT(4,NI,K) = sediment 2 transport velocity in m/s (F10.0)

TQ(4,NI,K) = time in days (F10.0)

Record 21 is repeated NBRKQ(4,NI)/4 times

Record 17 is input once for Data Block D4. Records 18, 19, 20 and 21 are input for each velocity time function. Record 19 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 21 uses as many lines as needed to input NBRKQ sets of QT and TQ with four sets per line.

DATA BLOCK D 5 Sediment 3 Transport Field

Sediment transport flow data are input as velocities and areas. Velocities may vary in time, and represent settling, sedimentation, deposition and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids 3 are modeled enter 0 for NINQ(5), then skip directly to the next data block.

Record 22--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(5) = number of velocity time functions for Field 5 (I5)

SCALQ = scaling factor for velocities (F10.0)

CONVQ = units conversion factor (F10.0)

Records 23 - 26 are input as a group NINQ(5) times

Record 23--Number of Segment Pairs (I5)

NOQS(5,NI) = number of segment pairs involved in sediment 3 transport (I5)

Record 24--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(5,NI,K) = area in square meters between segment pair K (F10.0)

JQ(5,NI,K) = segment sediment is transported from (I5)

IQ(5,NI,K) = segment sediment is transported to (I5)

Record 24 is repeated NOQS(5,NI)/4 times

Record 25--Number of Breaks in Velocity Time Function (I5)

NBRKQ(5,NI) = number of velocities and times used to describe piecewise linear time function NI (I5)

Record 26--Piecewise Linear Velocity Time Function (4(2F10.0))

✓ QT(5,NI,K) = sediment 3 transport velocity in m/s (F10.0)

TQ(5,NI,K) = time in days (F10.0)

Record 26 is repeated NBRKQ(5,NI)/4 times

Record 22 is input once for Data Block D5. Records 23, 24, 25 and 26 are input for each velocity time function. Record 24 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 26 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.

DATA BLOCK D6 Evaporation and Precipitation Field

Evaporation and precipitation flow data are input as velocities and areas. Velocities may vary in time to represent rainfall events or seasonal evaporation. No chemical is

~~transported with evaporation, but~~ volumes are adjusted to maintain continuity. If this field is not modeled, skip directly to Record 32 (Flow Bypass Options) After all transport field data are entered, Record 32 is input with NOSYS entries If no evaporation or precipitation fields are specified, Record 32 follows Data Group D 5 (solids 3 transport)

Record 27--Number of Velocity Time Functions (I5, 2F10.0))

NINQ(6) = number of velocity time functions for Field 6 (I5)

SCALQ = scaling factor for velocities (F10 0)

CONVQ = units conversion factor (F10 0)

Records 28 - 31 are input as a group NINQ(6) times

Record 28--Number of Segment Pairs (I5)

NOQS(6,NI) = number of segment pairs involved in evaporation or precipitation (I5)

Record 29--Areas for Evaporation, Precipitation (4(F10.0, 2I5))

BQ(6 NI K) = area in square meters between segment pair K (F10 0)

JQ(6,NI,K) = segment water is transported from, if = 0, this is precipitation (I5)

IQ(6 NI,K) = segment water is transported to, if = 0 this is evaporation (I5)

Record 29 is repeated NOQS(6,NI)/4 times

Record 30--Number of Breaks in Velocity Time Function (I5)

NBRKQ(6 NI) = number of velocities and times used to describe piecewise linear time function NI (I5)

Record 31--Piecewise Linear Velocity Time Function (4(2F10 0))

QT(6 NI K) = water transport velocity in m/s if more traditional units of cm/day or cm/year are desired, then specify CONVQ = 1 1574E^{7} or 3 169E^{10}, respectively (F10 0)

TQ(6,NI,K) = time in days (F10 0)

Record 31 is repeated NBRKQ(6,NI)/4 times

END OF DATA BLOCKS FOR D

Record 32--Flow Bypass Options (16I5)

QBY(ISYS) = flow bypass option -- 0 = flow transport occurs in system ISYS, 1 = flow transport is bypassed for system ISYS (I5)

ISYS = 1 NOSYS

The flow bypass option allows flow transport to be set to zero in one or more systems The bypass option applies to all transport fields

5 2 THE EXTERNAL HYDRODYNAMIC FILE

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ye

When IQOPT in Record 1 is set to 3 external flows and volumes will be read from a formatted ASCII file chosen by the user This file begins with information on the WASP5 calculational time step, simulation start and end times, and flow connections The body of the file is composed of sets of segment records and segment interface records that are repeated every time step for the entire simulation The segment records specify instantaneous segment volumes depths, and water velocities at the beginning of a time step The segment interface records specify average interfacial flows during the time step

WASP5 uses the interfacial flows to calculate mass transport, and the volumes to calculate constituent concentrations Segment depths and velocities are used only to calculate reaeration or volatilization rates

Five records comprise the external hydrodynamic file

Record 1 -- Data Options (2I5, 3F20 0, I5)

NQSEG = Number of segments connected by flows from the hydrodynamic file (I5)

NQINT = Number of interfacial flow pairs from the hydrodynamic file (I5)

DELTQ = WASP5 time step an even multiple of the hydrodynamic time step, seconds (F20.0)

TBEGIN = Beginning time for the hydrodynamic file, in seconds (F20.0)

TEND = Ending time for the hydrodynamic file, in seconds (F20.0)

FILOPT = Switch controlling the contents of the hydrodynamic file, 0 = time variable segment depths and velocities are read, 1 = time variable segment depths and velocities are not read (I5)

Record 2 -- Segment Interface Pairs (2I5)

IQ(J) = First segment in interface "J", nominally where flow is *from* (I5)

JQ(J) = Second segment in interface J nominally where flow is *to* (I5)

Note that positive values of flow go from IQ to JQ. Negative values of flow go from JQ to IQ

Record 2 is repeated NQINT times, for J from 1 to NQINT

Record 3 -- Initial Segment Properties (4F20.0)

BVOL(I) = Volume of segment 'I' at beginning of time step m^3 (F20.0)

DUMMY = Dummy variable not used by WASP5 (20.0)

DEPTH(I) = Average depth of segment I, in meters (F20.0)

VELOC = Average velocity of segment "I', m/sec (F20.0)

Record 3 is repeated NQSEG times for I from 1 to NQSEG

Records 4 and 5 are repeated as a unit for the number of time steps in the water quality simulation, or (TEND - TBEGIN)/DELTQ

Record 4 -- Segment Interfacial Flows (F20.0)

BQ(J) = Average flow in interfacial pair J during the time step, in m^3/sec (F20.0)

Record 4 is repeated NQINT times, for J from 1 to NQINT (in the same order as segment pairs are given in Record 2)

Record 5 -- Segment Properties (4F20.0)

BVOL(I) = Volume of segment "I" at end of time step, m^3 (F20 0)

DUMMY = Dummy variable, not used by WASP5 (20 0)

DEPTH(I) = Average depth of segment "I", in meters (F20 0)

VELOC = Average velocity of segment "I", m/sec (F20 0)

Record 5 is repeated NQSEG times, for I from 1 to NQSEG

Record 1 is input once Record 2 is repeated NQINT times Record 3 is repeated NQSEG times Records 4 and 5 are a set, and are repeated (as a set) (TEND - TBEGIN)/DELTQ times Within each set, Record 4 is repeated NQINT times and Record 5 is repeated NQSEG times

CHAPTER 6

DATA GROUP E   BOUNDARY CONCENTRATIONS

Data Group E supplies concentrations for each system at the model network boundaries Model boundaries consist of those segments that import, export, or exchange water with locations outside the network, as specified in Data Groups B and D All system concentrations from 1 to NOSEG must be supplied for each boundary. Boundary concentrations vary with time following a piecewise linear time function specified by the user in Records 3 and 4

6 1 RECORD FORMATS

Data Group E is repeated, in its entirety, NOSYS times

Record 1--Data Input Option--Number of Boundary Conditions (I10, 70X)

NOBC(K) = number of boundary conditions used for system K (I10)

TITLE = name of data group (70X)

If no boundary conditions are to be input for system K, set NOBC(K) equal to zero and either continue with the next system or go to Data Group F if K is the last system

Record 2--Scale Factor for Boundary Conditions (2F10.0)

SCALB = scale factor for boundary conditions All boundary conditions will be multiplied by this factor (F10 0)

CONVB = unit conversion factor for boundary conditions Boundary conditions are expected to be in milligrams per liter (mg/L) If boundary conditions are given in SI units (grams per cubic meter) CONVB will be 1 0 (F10 0)

Records 3-4 are input as a unit NOBC(K) times

Record 3--Boundary Conditions (2I5)

IBC(K) = boundary segment number (I5)

NOBRK(K) = number of values and times used to describe the broken line approximation The number of breaks must be equal for all boundary conditions within a system (I5)

Record 4--Boundary Concentrations (4(2F10.0))

BCT(K) = value of the boundary concentration at time T(K) in mg/L (F10 0)

T(K) = time in days If the length of the simulation exceeds T(NOBRK), the broken line approximation is repeated, starting at T(1), i e , the approximation is assumed to be periodic, with period equation to T(NOBRK) All break times must agree for all segments, i e T(1) must be the same for all boundaries, T(2) must be the same for all boundaries, etc (F10 0)

Record 4 is repeated NOBRK(K)/4 times

Records 1 and 2 are entered once Records 3 and 4 are a set and are repeated NOBC times Within each NOBC set, Record 3 is entered once and Record 4 is repeated until NOBRK entries are input Four entries (four BCT(K)-T(K) pairs) will fit on each 80-space line The whole group (Records 1 - 4) is repeated NOSYS times, once for each model system

6 2 THE EUTROPHICATION MODEL

When running EUTRO4 Data Group E is input 8 times once for each system For those systems being bypassed, the user may specify 0 for the number of boundary conditions, and skip to the next system

The user should be careful to note that boundary concentrations for system 4 phytoplankton are input as chlorophyll a, in μg/L These are transformed internally to phytoplankton carbon using the carbon to chlorophyll ratio, which is specified in Data Group H as constant 46

6 3 THE TOXIC CHEMICAL MODEL

When running TOXI4, Data Group E is input NOSYS times once for each system simulated NOSYS is specified in Data Group A and has a maximum value of 6 For those systems being bypassed the user may specify 0 for the number of boundary conditions, and skip to the next system

The user should be careful to note that all boundary concentrations are input in the standard WASP units of mg/L (even though the output concentrations for chemical are in units of µg/L)

CHAPTER 7

DATA GROUP F WASTE LOADS

Data Group F is composed of two blocks of data Data Block F1 contains the point source waste loads used in the model These loads vary with time following a piecewise linear time function specified by the user in Records 3 and 4 Following complete specification of point source loads, nonpoint source loads are read from Data Block F2, which is composed of only one record in the input dataset Nonpoint source loads vary with time in a daily step function read from an external loading file

7 1 RECORD FORMATS

Data Block F1 (records 1-4) is repeated in its entirety NOSYS times

Record 1--Data Input Option, No. of Forcing Functions (I10, 70X)

NOWK(ISYS) = number of forcing functions used for system ISYS Forcing functions may also be considered as sources (loads) or sinks of a water quality constituent If no forcing functions are to be input, set NOWK(ISYS) to zero and continue with next system or go to next data group (I10)

TITLE = name of data group (70X)

Record 2

SCALW = scale factor for forcing functions All forcing functions will be multiplied by this factor (F10 0)

CONVW = unit conversion factor for forcing functions Forcing functions are expected to be in kilograms per day If forcing functions are given in English units (pounds per day), this factor will be 0 4535 (F10 0)

Records 3-4 are input as a unit NOWK(ISYS) times

Record 3--Number of Point Sources (2I5)

IWK(K) = segment number that has forcing function BWK(K) (I5)

NOBRK(K) = number of breaks used to describe the forcing function approximation The number of breaks must be equal for all forcing functions within a system. (I5)

Record 4--Point Source Time Function (4(2F10.0))

WKT(K) = value of the forcing function at time T(K), in kg/day. (F10.0)

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic with period equal to T(NOBRK). All break times must agree for all segments, i.e., T(1) must be the same for all loads, T(2) must be the same for all loads, etc. (F10.0)

Record 4 is repeated NOBRK(ISYS)/4 times

Records 1 and 2 are input once. Records 3 and 4 are a set and are repeated (as a set) NOWK times. Within each set Record 3 is entered once and Record 4 is repeated until all NOBRK entries are entered. Four entries (WKT(K)-T(K) pairs) will fit on each 80-space line. The entire group (Records 1 - 4) is repeated NOSYS times, once for each system.

Data Block F2, record 5 is input once

Record 5--Nonpoint Source Load Option (I10)

LOPT = nonpoint source load option, a value of 0 means that no nonpoint sources will be read from an external file; a value of 1 will cause the model to read a set of loads from an external file. The user will be prompted by WASP5 to provide information on the external file. This file and its contents are described below. (I10)

7.2 THE EXTERNAL NONPOINT SOURCE FILE

When LOPT is set to 1, external nonpoint sources will be read from a formatted ASCII file chosen by the user. This file contains information on which WASP5 systems and segments receive nonpoint source loads and a record of the nonzero loads by system, segment, and day.

Six records comprise the nonpoint source file

Record 1--Data Options (A15, 3I5)

NPSMOD = Name or description of nonpoint source model or method of generation, this is echoed to the output file for the record (A15)

NUMSEG = Number of segments receiving nonpoint source loads (I5)

INTOPT = Interpolation option, 1 = step function (only one in code now) (I5)

NUMSYS = Number of WASP systems receiving nonpoint source loads (I5)

Record 2--Loading Segments (I5)

LSEG(I) = segment number receiving loads (I5)

Record 2 is repeated NUMSEG times

Record 3--Loading Systems (20I5)

LSYS(I) = WASP system numbers receiving loads (I5)

Record 4--System Descriptors (A15)

NAMESY(I) = Name or description of WASP systems receiving loads (A15)

Record 4 is repeated NUMSYS times

Records 5 and 6 are repeated as a unit for the number of days that nonzero loads occur

Record 5--Loading Days (F10 0)

LDAY = Time in days for the following nonzero load (F10 0)

Record 6--Nonpoint Source Loads (A15, 20F10 0)

NAMESY(I) = System name or description (not read in by WASP) (A15)

NPSWK(I J) = Nonpoint source loads for WASP system I at all loading segments J in the order presented in Record 2 Loads are in kg/day (20F1

Record 6 is repeated NUMSYS times

Record 1 is input once Record 2 is repeated NUMSEG times Record 3 is then input once Record 4 is repeated NUMSYS times Records 5 and 6 are a set and are repeated (as a set) NUMSYS times Within each set, Record 5 is entered once and Record 6 is repeated NUMSYS times

7 3 THE EUTROPHICATION MODEL

When running EUTRO4, Data Block F1 is input 8 times once for each system For those systems being bypassed, the user may specify 0 for the number of waste loads, and skip to the next system

The user should note that waste loads for system 4, phytoplankton, are input as phytoplankton carbon, in kg/day

7 4 THE TOXIC CHEMICAL MODEL

When running TOXI4, Data Block F1 is input NOSYS times, once for each system simulated NOSYS is specified in Data Group A and has a maximum value of 6 For those systems being bypassed the user may specify 0 for the number of waste loads, and skip to the next system

CHAPTER 8

DATA GROUP G. PARAMETERS

Parameters are spatially-variable characteristics of the water body. The definition of the parameters will vary depending upon the structure and kinetics of the systems comprising each model. The input format, however, is constant. The number of parameters that is specified in Record 1 must be input for each segment.

8.1 RECORD FORMATS

Record 1--Number of Parameters (I10, 70X)

NOPAM = number of parameters required by the model. If no parameters are to be input, set NOPAM to zero and go to Data Group H. (I10)

TITLE = name of data group. (70X)

Record 2--Scale Factors for Parameters (4(A5, I5, F10.0))

ANAME(ISC) = descriptive name for parameter ISC (A5)

ISC = parameter number identifying parameter (I5)

PSCAL(ISC) = scale factor for parameter ISC (F10.0)

Record 2 is repeated NOPAM/4 times

Records 3-4 are input as a unit NOSEG times

Record 3--Segment Number (I10)

ISG = segment number for the following parameter values (I10)

Record 4--Segment Parameters (4(A5, I5, F10.0))

PNAME(ISC) = an optional one to five alphanumeric character descriptive name for parameter PARAM(ISG,ISC) (A5)

ISC = parameter number identifying parameter (I5)

PARAM(ISEG,ISC) = the value of parameter ISC in segment ISG (F10.0)

Record 4 is repeated NOPAM/4 times

Record 1 is input once in Data Group G, occupying one line Record 2 has NOPAM entries Four entries will fit on one line, thus, Record 2 uses as many 80-space lines as needed to enter all NOPAM entries Records 3 and 4 are repeated NOSEG times once for each segment For each segment, Record 4 uses as many lines as needed to enter all NOPAM entries

8 2 THE EUTROPHICATION MODEL

Listed below are the 12 parameters available for EUTRO4 simulations Six representative levels of analysis were outlined in Table 1 For Level 1 and 2 analyses, only TMPSG, TMPFN, SOD1D, and SODTA (3, 4 9, and 11) need be specified Spatially-variable reaeration rate constants may be directly specified using REARSG (14) For Level 3 analysis, VELFN, FNH4, and TOTLIM (1, 7, and 13) may be added (DEPTH, VELFN and TOTLIM are used to compute reaeration if rate constant K2 is specified (Constant 82) then VELFN, REARSG, and TOTLIM can be omitted if parameter REARSG is specified, then VELFN and TOTLIM can be omitted) For analyses at Level 4 and above, all parameters should be considered

ISC	ANAME	Definition and Units
1	VELFN	Pointer to the time-variable velocity function to be used for ISEG The four velocity functions are defined by the user in data group I
2	SAL	Average salinity of ISEG, in g/L, used in calculation of DO saturation
3	TMPSG	Segment temperature multiplier (CC) TMPSG varies overspace and can be either actual temperature or a normalized function depending on the definition of TEMP TMPSG(ISEG) * TEMP(TMPFN(ISEG)) = STP the temperature of segment ISEG
4	TMPFN	(1 2 3 4) Flag designating the time-variable temperature function to be used for ISEG The four temperature functions are defined by the user in data group I
5	KESC	Segment extinction coefficient multiplier (m^{-1}) KESG varies over space and can be either an actual extinction coefficient or a normalized function,

		depending on the definition of KE KESG~~(ISEG) *~~ KE(KEFN'ISEG)) = Ke, the extinction coefficient ~~for segment ISEG~~
6	KEFN	Pointer designating the time variable extinction coefficient (KE) to be used for segment ISEG The five extinction coefficients available are defined in data group I
7	FNH4	Average ammonium flux multiplier for segment (mg/m^2-day)
△8	FPO4	Average phosphate flux multiplier for segment (mg/m^2-day)
△9	SOD1D	Sediment oxygen demand for segment (g/m^2-day)
10-11	RLGHTS	Used internally not specified by the user
12	SODTA	Segment specific temperature correction coefficient (theta) for sediment oxygen demand
13	TOTLIM	Segment specific percent shading ?
14	REARSG	Segment specific reaeration rate constant multiplier, used in combination with time function REAR

8 3 THE TOXIC CHEMICAL MODEL

not used yet

Listed below are the 18 parameters that may be used by TOXI4 The user need input only those required to model the particular reactions being considered For solids, equilibrium, and kinetics Level 1, no parameters are necessary

ISC	ANAME	Definition, Units and Reactions Affected
1	VELFN	Pointer to water velocity time function (1-4), V
2	TMPFN	Pointer to normalized temperature time function (1-4), ALL
3	TEMP	Multiplier for water temperature time function (°C), ALL
4	WVEL	Multiplier for wind velocity (10 meters above segment surface) time function (meters/sec) V

ISC	ANAME	Definition, Units and Reactions Affected
5	REAR	Multiplier of time function 5, whose definition depends on volatilization option XV (constants 236 736,1336) XV = 1 volatilization rate constant (m/day) XV = 2,3 oxygen reaeration rate constant (m/day) XV = 4,5 REAER not used, enter 0, V
6	DOC	Dissolved organic carbon concentrations (mg/L) S, P
7	FOC 1	Fraction organic carbon of solids class 1, S
8	FOC 2	Fraction organic carbon of solids class 2, S
9	FOC 3	Fraction organic carbon of solids class 3, S
10	CHPHL	Multiplier for phytoplankton chlorophyll concentration time function (mg/L), P
11	PH	Multiplier for pH time function, H, I
12	XKE2	Light extinction coefficient for photochemically active light (1/meter), this value is used only for photolysis option XPHOTO = 2 (constants 286 886 1486) For photolysis option 1 or 2 when XKE2 = 0 0 the extinction coefficient is calculated from solids, DOC, and chlorophyll concentrations P
13	OXRAD	Concentration of oxidants, such as O_3 for H_2O_2 (moles/L) O
14	BAC	Density of active bacteria (cells/100 cc) the units for bacterial density must be consistent with those used for the second order biodegradation rate constants KBIO20 (constants 146-160, 746-760 1346-1360), the product of BAC and KBIO20 must be units of day^{-1} B
15	EXENV	Property of aquatic environment that affects the user-defined extra reaction The units for EXENV must be consistent with those used for second order rate constants KE20 (constant 576-590, 1176-1190, 1776-1790), the product of EXENV and KE20 must yield units of day^{-1}, E
16	TOTKG 1	Total lumped first-order decay rate constant for chemical 1 in segment (day^{-1})
17	TOTKG 2	Total lumped first-order decay rate constant for chemical 2 in segment (day^{-1})
18	TOTKG 3	Total lumped first-order decay rate for chemical 3 in segment (day^{-1})

I = ionization, S = sorption, V = volatilization B = biodegradation H = hydrolysis O = oxidation P = photolysis E = extra reaction

For equilibrium level 2, FOC 1 is used to enter partition coefficients For equilibrium levels 3 and above, FOC 1 is fraction organic carbon of solids class 1 DOC may be entered If two or three solids classes are being simulated (solids level 4) then FOC 2 and FOC 3 must be entered For equilibrium level 5, PH values are necessary

At kinetics level 2, TOTKG 1 is specified If two or three chemicals are being simulated at this level, then TOTKG 2 and TOTKG 3 must be specified Kinetics level 3 may require the remaining parameters, depending on the kinetic processes of importance If water temperatures differ significantly from 20°C, then TEMP may be necessary for all processes (depending on the accuracy required of the simulation) Volatilization requires REAR for options 1, 2 and 3, but not for 4 and 5 If reareation values are not available for volatilization options 2 and 3, then rates can be calculated internally if parameters DEPTH and VELOC are given Volatilization options 4 and 5 require parameter WVEL

Photolysis requires DEPTH values In addition photolysis option 1 requires DOC and CHPHL Photolysis option 2 may use either DOC and CHPHL values or XKE2 values The remaining processes of hydrolysis, oxidation biodegradation, and extra reaction require one parameter each PH, OXRAD, BAC, and EXENV, respectively

CHAPTER 9

DATA GROUP H CONSTANTS

The definition of the constants will vary, depending upon the structure and kinetics of the systems comprising each model This data group is subdivided into global constants and constants for each system (thus NOSYS+1 groups are read) Each of these groups can be subdivided into any number of fields containing similar kinds of data

9 1 RECORD FORMATS

Record 1--Header (80X)

TITLE = name of data group (80X)

Records 2-4 are input as a group NOSYS+1 times

Record 2--Data Fields in Group ISYS (A10, I10)

CHNAME(ISYS) = a ten-character descriptive name for System (ISYS) (A10)

NFLD = number of fields of constants for this group 0 = no constants for this group the user may subdivide the constants into any number of arbitrary fields (I10)

If no constants are to be input for this group set NFLD equal to zero and continue with next group Records 3 and 4 are repeated as a unit NFLD times

Record 3--Number of Constants in Field (A10, I10)

FLDNAME = ten-character name identifying field of constants (A10)

NCONS = number of constants to be entered in this field 0 = no constants for this field (skip to next field) (I10)

Record 4--Constants (2(A10, I10, F10.0))

TNAME(ISC) = name identifying constant ISC (A10)

ISC = number identifying constant, these numbers are set by model developer (I10)

CONST(ISC) = value of constant ISC (F10 0)

Record 4 is repeated NCONS/2 times

Record 1 is entered once in Data Group H Records 2 through 4 are entered as NOSYS + 1 groups For each group, Records 3 and 4 are entered NFLD times For each field, Record 4 uses as many lines as needed for NCONS entries (2 per line)

9 2 THE EUTROPHICATION MODEL

Listed below are the 42 constants available for a full eutrophication simulation Chapters 4 and 5 discuss the constants required for each level of complexity in dissolved oxygen and eutrophication modeling Default values for constants are 0 unless otherwise noted

ISC	ANAME	Definition and Units
11	K12C	Nitrification rate at 20蚓|, per day ?
12	K12T	Temperature coefficient for K1320C Default = 1 0
13	KNIT	Half-saturation constant for nitrification-oxygen limitation mg O_2/L
21	K20C	Denitrification rate at 20蚓|, per day ?
22	K20T	Temperature coefficient for K140C K20? Default = 1 0
23	KNO3	Half-saturation constant for denitrification oxygen limitation mgO_2/L
41	K1C	Saturated growth rate of phytoplankton (day^{1})
42	K1T	Temperature coefficient Default = 1 0
43	LGHTS ?	Light formulation switch LGHTS = 1 use Di Toro et al (1971) formulation LGHTS = 2, use Dick Smith's (USGS) formulation Default = 1
44	PHIMX	Maximum quantum yield constant Used only when LGHTS = 2, mg C/mole photons Default = 720 ?
45	XKC	Chlorophyll extinction coefficient Used only when LGHTSW = 2, (mg chla/m')^{1}/m Default =

0 017

46	CCHL	Carbon-to-chlorophyll ratio Used only when LGHTSW = 1 (mg carbon/mg chl **a**) Default = 30
47	IS1	Saturation light intensity for phytoplankton Used only when LGHTSW = 1 (Ly/day) Default = 300
48	KMNG1	Nitrogen half-saturation constant for nitrogen for phytoplankton growth, which also affects ammonia preference, mg-N/L NOTE This affects ammonia preference 0 2 (0 05) = 0, PNH3G1 = 1 0 = Large, PNH3G1 = $NH_3/(NH_3 + NO_3)$ NOTE For standard model application, use a large KMNG1
49	KMPG1	Phosphorous half-saturation constant for phytoplankton growth mg PO_4-P/L 0 02~0 08 0 01~1/5
50	K1RC	Endogenous respiration rate of phytoplankton at 20°C day^{1} 0 05~0 15
51	K1RT	Temperature coefficient for phytoplankton respiration Default = 1 0
52	K1D	Non-predatory phytoplankton death rate, day^{1} 0 003~0 17
53	K1G	Grazing rate on phytoplankton per unit zooplankton population, L/cell-day 0 1~1 5
54	NUTLIM	Nutrient limitation option 0 = minimum, 1 = multiplicative Default = 0
55	KPZDC	Decomposition rate constant for phytoplankton in the sediment at 20°C, per day
56	KPZDT	Temperature coefficient for decomposition of phytoplankton in sediment Default = 1 0
57	PCRB	Phosphorus-to-carbon ratio in phytoplankton, mg P/mg C Default = 0 025
58	NCRB	Nitrogen-to-carbon ratio in phytoplankton, mg N/mg C Default = 0 25
59	KMPFY	Half-saturation constant for phytoplankton, mg carbon/L NOTE As phytoplankton concentrations

0 5~0 6

Jorgensen et al 1978

		increase, mineralization rates for organic nitrogen and organic phosphorus increase If KMPHY is small, there is little phytoplankton effect on mineralization If KMPHY is large, a large concentration of phytoplankton is needed to drive mineralization For standard model application, use KMPHYT = 0
71	KDC	CBOD deoxygenation rate at 20蚓|, per day
72	KDT	Temperature coefficient for carbonaceous deoxygenation in water column Default = 1 0
73	KDSC	Decomposition rate of carbonaceous BOD in the sediment at 20蚓|, per day
74	KDST	Temperature coefficient for carbonaceous deoxygenation in the sediment Default = 1 0
75	KBOD	Half saturation constant for carbonaceous deoxygenation oxygen limitation
81	OCRB	Oxygen to carbon ratio in phytoplankton, mg O_2/mg C Default = 32/12
82	K2	Reaeration rate constant at 20蚓| for entire water body, day NOTE If K2 is not entered, the reaeration rate will be calculated as the product of parameter REARSG and time function REAR If parameter REARSG is not entered the reaeration rate will be calculated from water velocity, depth, and wind velocity
91	K71C	Mineralization rate of dissolved organic nitrogen per day
92	K71T	Temperature coefficient for K1013C Default = 1 0
93	KONDC	Decomposition rate constant for organic nitrogen in the sediment at 20蚓|, per day
94	KONDT	Temperature coefficient for decomposition of organic nitrogen in the sediment Default = 1 0
95	FON	Fraction of dead and respired phytoplankton nitrogen recycled to organic nitrogen Default = 1 0
100	K83C	Mineralization rate of dissolved organic

		phosphorus, per day
101	K83T	Temperature coefficient for K58C Default = 1 0
102	KOPDC	Decomposition rate of organic phosphorus in the sediment at 20°C, per day
103	KOPDT	Temperature coefficient for decomposition of organic phosphorus in the sediment Default = 1 0
104	FOP	Fraction of dead and respired phytoplankton phosphorus recycled to organic phosphorus Default = 1 0

9 3 THE TOXIC CHEMICAL MODEL

not read 08/12/91

A large number of constants are available to characterize the various chemical reactions at different levels of complexity Very few need be specified for any one simulation Table 3 summarizes the constants that may be used for equilibrium and kinetics level 1 Only two of these need be specified--PIXC(1 1) and either a half life or a first order rate constant For equilibrium and kinetics level 2 no constants need be specified--partition coefficients and rate constants are entered via parameters

For kinetics level 3, some general chemical constants are usually available, as summarized in Table 4 MOLWT, SOLG and VAPRG are sometimes used in volatilization computations, while LKOW can be used in sorption calculations

If a chemical is ionic then constants from Table 5 may be specified For each ionic specie I, SPFLG(I) and PKA(I) must be specified EPKA(I) may also be given Ionic speciation is considered to be equilibrium level 5 The presence of ionic species requires significantly more data specifications for the remaining processes

Hydrophobic sorption at equilibrium levels may be simulated with constants from Table 6 If LKOC is unknown then LKOW, A0 and A1 should be specified (if A0 and A1 are unknown, they default to log 0 6 and 1, respectively) NUX(1) and PIXC(I,1) should be left out Solids-dependent partitioning constitutes equilibrium level 4 NUX(1) should be given a value of around 1 For equilibrium level 5, ionic sorption constants must also be specified Their locations are given in Table 7

For kinetics level 3, constants must be specified for each relevant process Constants for volatilization, biodegradation, alkaline hydrolysis, neutral hydrolysis, acid hydrolysis, oxidation, and photolysis are given in Tables 8, 9, 11, 13, 15, 17, 19, and 20, respectively Constants for a user-specified extra reaction are given in Table 22 If ionic speciation is being considered, then ionic rate constants must also be specified for each existing ionic specie Locations of these constants are given in Tables 10, 12, 14, 16, 18, 21 and 23

For kinetics level 4, reaction products are simulated Four cases are illustrated in Figure 6 1 (in Part A of this manual) Yield coefficients for each relevant process must be specified Yield coefficients for chemical 1, 2, and 3 reactions are listed in Tables 24, 25, and 26 The reactions themselves need not be second order to simulate reaction products

TABLE 3 CONSTANTS FOR SIMPLE TOXI4 REACTIONS

Constant Number			Variable	Definition
C_1	C_2	C_3		
111	711	1311	PIXC(1,1)	Constant partition coefficient for sorption to solids (class 1), l_w/kgs
			K_1	First order loss rate constants, day ^{1}
140	740	1340	KV	Volatilization
141	741	1341	KBW	Water column biodegradation
142	742	1342	KBS	Benthic biodegradation
181	781	1381	KHOH	Alkaline hydrolysis
182	782	1382	KHN	Neutral hydrolysis
183	783	1383	KHH	Acid hydrolysis
256	856	1456	KO	Oxidation
287	887	1487	KF	Photolysis
571	1171	1771	KE	Extra reaction
			TH_1	Half lives for reactions day
143	743	1343	THBW	Water column biodegradation
144	744	1344	THBS	Benthic biodegradation
252	852	1452	THHOH	Alkaline hydrolysis
253	853	1453	THHN	Neutral hydrolysis
254	854	1454	THHH	Acid hydrolysis
257	857	1457	THO	Oxidation
289	889	1489	THF	Photolysis
572	1172	1772	THE	Extra reaction

TABLE 4 GENERAL CHEMICAL CONSTANTS

Constant Number			Variable	Definition
C_1	C_2	C_3		
9	609	1209	TDINT	Time interval at which rate constants are recomputed, days
81	681	1281	MOLWT	Molecular weight, g/mole
82	682	1282	SOLG	Solubility, mg/L
83	683	1283	VAPRG	Vapor pressure, torr
84	684	1284	LKOW	Log octanol-water partition coefficient, L_o/L_w

TABLE 5 IONIZATION CONSTANTS

Constant Number C_1	C_2	C_3	Variable	Definition
85	685	1285	SFLG(1)	flags indicating existence of ionic species +, ++, -, --, if SPFLG(I) = 1, ionic species I exists
86	686	1286	SFLG(2)	
87	687	1287	SFLG(3)	
88	688	1288	SFLG(4)	
91	691	1291	PKA(1)	For ionic species I, the constant in the integrated Van't Hoff equation describing temperature dependence of the equilibrium dependence of the equilibrium constant for dissociation log K(I) = -PKA(I) + (EPKA(I)/2 303 R) * [$T*T_P/(T-T_R)$]
92	692	1292	PKA(2)	
93	693	1293	PKA(3)	
94	694	1294	PKA(4)	
95	695	1295	EPKA(1)	For ionic species I, the activation energy of the dissociation reaction, kcal/mole
96	696	1296	EPKA(2)	
97	697	1297	EPKA(3)	
98	698	1298	EPKA(4)	
99	699	1299	TREFI	Reference temperature at which dissociation reaction constants were measured, 蚓

TABLE 6 SORPTION CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
84	684	1284	LKOW	Log 10 of the octanol-water partition coefficient, log (L_w/L_o)
101	701	1301	LKOC	Log 10 of the organic carbon partition coefficient, log (L_w/kg_{oc})
102	702	1302	A0	Intercept in the K_{ow} - K_{oc} correlation log K_{oc} = A0 · log K_{ow}, default = log 0 6
103	703	1303	A1	Slope in the K_{ow} - K_{oc} correlation, default = 1 0
106	706	1306	NUX(1)	Solids-dependent partitioning parameter (υ_x) of the chemical onto solids, default = 10^{12} makes K_p independent of solids concentration
111	711	1311	PIXC(1,1)	Solids-independent (limiting) partition coefficient K_{po} for sorption to solid 1, L_w/kg_s
116	716	1316	PIXC(2,1)	Solids-independent (limiting) partition coefficient K_{po} for sorption to solid 2 L_w/kg_s
121	721	1321	PIXC(3 1)	Solids-independent (limiting) partition coefficient K_{po} for sorption to solid 3, L_w/kg_s If = 0, K_{po} for neutral chemical will be calculated from LKOC and parameter FOC
--	--	--	PIDOC	Partition coefficient for DOC, for neutral chemical KOC is used L/kg

TABLE 7 LOCATION OF IONIC SORPTION CONSTANTS

Constant Number			Variable	Ionic Specie	Sorptive Phase
C_1	C_2	C_3			
106	706	1306	NUX(1)	0	S
107	707	1307	NUX(2)	+	S
108	708	1308	NUX(3)	++	S
109	709	1309	NUX(4)	-	S
110	710	1310	NUX(5)	--	S
111	711	1311	PIXC(1,1)	0	S1
112	712	1312	PIXC(1,2)	+	S1
113	713	1313	PIXC(1,3)	++	S1
114	714	1314	PIXC(1 4)	-	S1
115	715	1315	PIXC(1,5)	--	S1
116	716	1316	PIXC(2,1)	0	S2
117	717	1317	PIXC(2,2)	+	S2
118	718	1318	PIXC(2,3)	++	S2
119	719	1319	PIXC(2 4)	-	S2
120	720	1420	PIXC(2,5)	--	S2
121	721	1421	PIXC(3,1)	0	S3
122	722	1422	PIXC(3 2)	+	S3
123	723	1423	PIXC(3,3)	++	S3
124	724	1424	PIXC(3,4)	-	S3
125	725	1425	PIXC(3,5)	--	S3
126	726	1426	PIDOC(1)	+	B
127	727	1427	PIDOC(2)	++	B
128	728	1428	PIDOC(3)	-	B
129	729	1429	PIDOC(4)	--	B

TABLE 8 VOLATILIZATION CONSTANTS

Constant Number				
C_1	C_2	C	Variable	Definition
136	736	1336	XV	Volatilization option 0 = no volatilization 1 = measured volatilization 2 = measured reaeration + O'Conner for gas transfer 3 = measured reaeration + MacKay for gas transfer 4 = calculated using O'Conner 5 = calculated using MacKay
137	737	1337	HENRY	Henry's constant atm-m^3/mole
138	738	1338	KLT	Volatilization temperature correction factor, dimensionless
139	739	1339	KVOG	Measured ratio of volatilization to reaeration rates
2	2	2	WTYPE	Water body type (0 = flowing stream, river, or estuary, 1 = stagnant pond or lake)
5	5	5	AIRTMP	Multiplier for air temperature time function
8	608	1208	ATMOS	Atmospheric concentration of chemical, 痢/L

TABLE 9 SECOND ORDER BIODEGRADATION CONSTANTS FOR TOTAL FOR NEUTRAL CHEMICAL

Constant Number C_1	C_2	C_3	Variable	Definition
146	746	1346	KBIO20(1,1)	Second-order 20°C biodegradation rate constant for aqueous, DOC-sorbed, and sediment-sorped phases, mL/cells-day
151	751	1351	KBIO20(2,1)	
156	756	1356	KBIO20(3,1)	
161	761	1361	Q10DIS(1)	Temperature correction factor for biodegradation of aqueous, DOC-sorbed, and sediment-sorbed phases, multiplication factor for 10°C temperature increase
166	766	1366	Q10DOC(1)	
171	771	1371	Q10PAR(1)	

TABLE 10 LOCATION OF IONIC BIODEGRADATION CONSTANTS

Constant Number			Variable	Ionic Specie	Sorptive Phase
C	C_2	C_3			
146	746	1346	KBIO20(1,1)	0	W
147	747	1347	KBIO20(1,2)	+	W
148	748	1348	KBIO20(1,3)	++	W
149	749	1349	KBIO20(1,4)	-	W
150	750	1350	KBIO20(1,5)	--	W
151	751	1351	KBIO20(2,1)	0	B
152	752	1352	KBIO20(2,2)	+	B
153	753	1353	KBIO20(2 3)	++	B
154	754	1354	KBIO20(2,4)	-	B
155	755	1355	KBIO20(2 5)	--	B
156	756	1356	KBIO20(3,1)	0	S
157	757	1357	KBIO20(3 2)	+	S
158	758	1358	KBIO20(3,3)	++	S
159	759	1359	KBIO20(3,4)	-	S
150	760	1460	KBIO20(3,5)	--	S
161	761	1461	Q10DIS(1)	0	W
162	762	1462	Q10DIS(2)	+	W
163	763	1463	Q10DIS(3)	++	W
164	764	1464	Q10DIS(4)	-	W
165	765	1465	Q10DIS(5)	--	W
166	766	1466	Q10DOC(1)	0	B
167	767	1467	Q10DOC(2)	+	B
168	768	1468	Q10DOC(3)	++	B
169	769	1469	Q10DOC(4)	-	B
170	770	1470	Q10DOC(5)	--	B
171	771	1471	Q10PAR(1)	0	S
172	772	1472	Q10PAR(2)	+	S
173	773	1473	Q10PAR(3)	++	S
174	774	1474	Q10PAR(4)	-	S
175	775	1475	Q10PAR(5)	--	S

TABLE 11 SECOND ORDER ALKALINE HYDROLYSIS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
184	784	1384	TREFH	Reference temperature at which hydrolysis rates were measured, 蚓
186	786	1386	KH2O(1,1,1)	Second order, 20蚓 alkaline hydrolysis rate constants for aqueous, DOC-sorbed , and sediment-sorbed phases, L/mole-day
191	791	1391	KH2O(1 2 1)	
196	796	1396	KH2O(1 3 1)	
231	831	1431	EHOH(1)	Activation energy for alkaline hydrolysis, kcal/mole

TABLE 12 LOCATION OF IONIC ALKALINE HYDROLYSIS CONSTANTS

Constant Number			Variable	Ionic Specie	Sorptive Phase
C_1	C_2	C_3			
186	786	1386	KH2O(1,1,1)	0	W
187	787	1387	KH2O(1,1,2)	+	W
188	788	1388	KH2O(1,1,3)	++	W
189	789	1389	KH2O(1,1,4)	-	W
190	790	1390	KH2O(1 1,5)	--	W
191	791	1391	KH2O(1,2,1)	0	B
192	792	1392	KH2O(1,2,2)	+	B
193	793	1393	KH2O(1,2 3)	++	B
194	794	1394	KH2O(1,2,4)	-	B
195	795	1395	KH2O(1,2 5)	--	B
196	796	1396	KH2O(1,3,1)	0	S
197	797	1397	HK2O(1,3,2)	+	S
198	798	1398	KH2O(1,3,3)	++	S
199	799	1399	KH2O(1 3 4)	-	S
200	800	1400	KH2O(1,3,5)	--	S
231	831	1431	EHOH(1)	0	A
232	832	1432	EHOH(2)	+	A
233	833	1433	EHOH(3)	++	A
234	834	1434	EHOH(4)	-	A
235	835	1435	EHOH(5)	--	A

TABLE 13 SECOND ORDER NEURAL HYDROLYSIS CONSTANTS FOR TOTAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
184	784	1384	TREFH	Reference temperature at which hydrolysis rates were measured 蚓
201	801	1401	KH2O(2,1,1)	20蚓 neutral hydrolysis rate constant for aqueous, DOC-sorbed, and sediment-sorbed phases, day^{1}
206	806	1406	KH2O(2,2,1)	
211	811	1411	KH2O(2,3,1)	
236	836	1436	EHN(1)	Activation energy for neutral hydrolysis kcal/mole

TABLE 14 LOCATION OF IONIC NEUTRAL HYDROLYSIS CONSTANTS

Constant Number			Variable	Ionic Specie	Sorptive Phase
C_1	C_2	C_3			
201	801	1401	KH2O(1,1,2)	0	W
202	802	1402	KH2O(2,1,2)	+	W
203	803	1403	KH2O(3,1,2)	++	W
204	804	1404	KH2O(4,1,2)	-	W
205	805	1405	KH2O(5,1,2)	--	W
206	806	1406	KH2O(1,2,2)	0	B
207	807	1407	KH2O(2,2,2)	+	B
208	808	1408	KH2O(3,2,2)	++	B
209	809	1409	KH2O(4,2,2)	-	B
210	810	1010	KH2O(5,2 2)	--	B
211	811	1411	KH2O(1,3,2)	0	S
212	812	1412	KH2O(2,3,2)	+	S
213	813	1413	KH2O(3,3,2)	++	S
214	814	1414	KH2O(4,3,2)	-	S
215	815	1415	KH2O(5,3,2)	--	S
236	836	1436	EHN(1)	0	A
237	837	1437	EHN(2)	+	A
238	838	1438	EHN(3)	++	A
239	839	1439	EHN(4)	-	A
240	840	1440	EHN(5)	--	A

TABLE 15 SECOND ORDER ACID HYDROLYSIS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
184	784	1384	TREFH	Reference temperature at which hydrolysis rates were measured, 蚓
216	816	1416	KH2O(3,1,1)	Second order, 20蚓 acid hydrolysis rate constant for aqueous, DOC-sorbed and sediment-sorbed phases, L/mole-day
221	821	1421	KH2O(3,2,1)	
226	826	1426	KH2O(3 3,1)	
241	841	1441	EHH(1)	Activation energy for aced hydrolysis kcal/mole

TABLE 16 LOCATION OF IONIC ACID HYDROLYSIS CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
216	816	1416	KH2O(3,1,1)	0	W
217	817	1417	KH2O(3,1,2)	+	W
218	818	1418	KH2O(3,1,3)	++	W
219	819	1418	KH2O(3,1,4)	-	W
220	820	1420	KH2O(3,1,5)	--	W
221	821	1421	KH2O(3,2,1)	0	B
222	822	1422	KH2O(3,2,2)	+	B
223	823	1423	KH2O(3,2,3)	++	B
224	824	1424	KH2O(3,2,4)	-	B
225	825	1425	KH2O(3,2,5)	--	B
226	826	1426	KH2O(3,3,1)	0	S
227	827	1427	KH2O(3,3,2)	+	S
228	828	1428	KH2O(3,3,3)	++	S
229	829	1429	KH2O(3,3,4)	-	S
230	830	1430	KH2O(3,3,5)	--	S
241	841	1441	EHH(1)	0	A
242	842	1442	EHH(2)	+	A
243	843	1443	EHH(3)	++	A
244	844	1444	EHH(4)	-	A
245	845	1445	EHH(5)	--	A

TABLE 17 SECOND ORDER OXIDATION CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
258	858	1458	TREFO	Reference temperature at which oxidation rates were measured 蚓
261	861	1461	KOX2O(1,1)	Second-order, 20蚓 oxidation rate constant for aqueous, DOC-sorbed, and sediment_sorbed phases, L/mole-day
266	866	1466	KOX2O(2,1)	
271	871	1471	KOX2O(3 1)	
276	876	1476	EOX(1)	Activation energy for oxidation, kcal/mole

TABLE 18 LOCATION OF IONIC OXIDATION CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
261	861	1461	KOX2O(1,1)	0	W
262	862	1462	KOX2O(2,1)	+	W
263	863	1463	KOX2O(3,1)	++	W
264	864	1464	KOX2O(4,1)	-	W
265	865	1465	KOX2O(5,1)	--	W
266	866	1466	KOX2O(1,2)	0	B
267	867	1467	KOX2O(2,2)	+	B
268	868	1468	KOX2O(2,2)	++	B
269	869	1469	KOX2O(4 2)	-	B
270	870	1470	KOX2O(5,2)	--	B
271	871	1471	KOX2O(1,3)	0	S
272	872	1472	KOX2O(2,3)	+	S
273	873	1473	KOX2O(3,3)	++	S
274	874	1474	KOX2O(4,3)	-	S
275	875	1475	KOX2O(5,3)	--	S
276	876	1476	EOX(1)	0	All
277	877	1477	EOX(2)	+	All
278	878	1478	EOX(3)	++	All
279	879	1479	EOX(4)	-	All
280	880	1480	EOX(5)	--	All

TABLE 19 TOXI4 PHOTOLYSIS CONSTANTS

Constant Number				
C_1	C_2	C_3	Variable	Definition
286	886	1486	XPHOTO	Photolysis option 0 = no photolysis, 1 = computed from absorptivity, 2 = measured surface rate
288	888	1488	RFLATG	Latitude at which surface photolysis rate was measured, degree and tenths (option 2)
291	891	1491	KDPG(1)	Measured surface photolysis rate for neutral specie, day^{-1} (option 2)
296	896	1496	LAMAXG(1)	Wavelength of maximum light absorption for neutral specie, nm (option 2)
301-346	901-946	1501-1546	ABS(K,1,L)	Molar absorptivity of neutral specie of chemical K at wavelength number L L/mole-cm-ln10 (option 1)
551	1151	1751	QUANTG(1 1)	Quantum yield of dissolved neutral chemical
556	1156	1756	QUANTG(1,2)	Quantum yield of dissolved neutral chemical
561	1161	1761	QUANTG(3,1)	Quantum yield of dissolved neutral chemical

L = Wavelength 1-46 (see Tables 7 12 and 7 13 in Part A of this document)

TABLE 20 GLOBAL CONSTANTS FOR TOXI4 PHOTOLYSIS OPTION 1

Constant Number				
C_1	C_2	C_3	Variable	Definition
1	601	1201	TO	Julian date at beginning of run
3	603	1203	ELEVG	Average ground surface elevation, m
4	604	1204	LATG	Latitude of water body, degrees
6	606	1206	XLITE	Water surface light intensity option, 0 = do not compute light, 1 = annual average, 2 = average for month indicated by TO, 3 = monthly step function
7	607	1207	DFACG	Ratio of optical path length to vertical depth, 1 17
11-23	611-623	1211-1223	CLOUDG(1)	Mean monthly cloudiness, in tenths of full sky coverage (0-10)
24-36	624-636	1224-1236	AIRTYG(1)	Mean monthly air mass type 1 = rural, 2 = urban, 3 = maritime, 4 = tropospheric
37-49	637-649	1237-1249	RHUMG(1)	Mean monthly daylight relative humidity percent
50-62	650-662	1250-1262	ATURBG(1)	Mean monthly atmospheric turbidity, in equivalent aerosol layer thickness km
63-75	663-675	1263-1275	OZONEG(1)	Mean monthly ozone content of atmosphere, in cm NTP (0 2 - 0 3)

TABLE 21 LOCATION OF IONIC PHOTOLYSIS CONSTANTS

Constant Number			Variable	Ionic Specie	Sorptive Phase
C_1	C_2	C_3			
291	891	1491	KDPG(1)	0	A
292	892	1492	KDPG(2)	+	A
293	893	1493	KDPG(3)	++	A
294	894	1494	KDPG(4)	-	A
295	895	1495	KDPG(5)	--	A
296	896	1496	LAMAXG(1)	0	A
297	897	1497	LAMAXG(2)	+	A
298	898	1498	LAMAXG(3)	++	A
299	899	1499	LAMAXG(4)	-	A
300	900	1500	LAMAXG(5)	--	A
301-346	901-946	1501-1546	ABS(K 1 L)	0	A
351-396	951-996	1551-1596	ABS(K 2 L)	+	A
401-446	1001-1046	1601-1646	ABS(K 3,L)	++	A
451-496	1051-1096	1561-1696	ABS(K,4,L)	-	A
501-546	1101-1146	1701-1746	ABS(K 5,L)	--	A
551	1151	1751	QUANTG(1 1)	0	W
552	1152	1752	QUANTC(1 2)	++	W
553	1153	1753	QUANTC(1,3)	+	W
554	1154	1754	QUANTG(1,4)	-	W
555	1155	1755	QUANTC(1,5)	--	W
556	1156	1756	QUANTG(2,1)	0	B
557	1157	1757	QUANTG(2,2)	+	B
558	11458	1758	QUANTG(2 3)	++	B
559	1159	1759	QUANTG(2 4)	-	B

TABLE 21 LOCATION OF IONIC PHOTOLYSIS CONSTANTS

Constant Number			Variable	Ionic Specie	Sorptive Phase
C_1	C_2	C_3			
560	1160	1760	QUANTG(2,5)	--	B
561	1161	1761	QUANTG(3,1)	0	S
562	1162	1762	QUANTG(3,2)	++	S
563	1163	1763	QUANTG(3 3)	+	S
564	1164	1764	QUANTG(3,4)	-	S
565	1165	1765	QUANTG(3,5)	--	S

TABLE 22 EXTRA SECOND ORDER REACTIONS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
573	1173	1773	TREFE	Reference temperature at which extra reaction rates were measured 蚓
576	1176	1776	KE2O(1,1)	Second-order, 20蚓 extra reaction rate constant for aqueous, DOC-sorbed, and sediment-sorbed phases, 1/[E]-day
581	1181	1781	KE2O(2 1)	
586	1186	1786	KE2O(3,1)	
591	1191	1791	EEX(1)	Activation energy for extra reaction kcal/mole

TABLE 2 5 23 LOCATION OF IONIC EXTRA REACTION CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
576	1176	1776	KE2O(1,1)	0	W
577	1177	1777	KE2O(1,2)	+	W
578	1178	1778	KE2O(1,3)	++	W
579	1179	1779	KE2O(1,4)	-	W
580	1180	1780	KE2O(1,5)	--	W
581	1181	1781	KE2O(2,1)	0	B
582	1182	1782	KE2O(2,2)	+	B
583	1183	1783	KE2O(2,3)	++	B
584	1184	1784	KE2O(2,4)	-	B
585	1185	1785	KE2O(2,5)	--	B
586	1186	1786	KE2O(3,1)	0	S
587	1187	1787	KE20(3,2)	+	S
588	1188	1788	KE2O(3,3)	++	S
589	1189	1789	KE2O(3,4)	-	S
590	1190	1790	KE2O(3,5)	--	S
591	1191	1791	EEX(1)	0	All
592	1192	1792	EEX(2)	+	All
593	1193	1793	EEX(3)	++	All
594	1194	1794	EEX(4)	-	All
595	1195	1795	EEX(5)	--	All

TABLE 24 YIELD CONSTANTS FOR CHEMICAL 1 REACTIONS

Constant Number				
C_1	C_2	C_3	Variable	Definition
			Y( )12	Yield coefficient for production of C_2 from C_1, mgC_2/mgC_1
176			YBW12	Water column biodegradation
178			YBS12	Benthic biodegradation
246			YHOH12	Alkaline hydrolysis
248			YHN12	Neutral hydrolysis
250			YHH12	Acid hydrolysis
281			YOX12	Oxidation
566			YF12	Photolysis
596			YE12	Extra reaction
			Y( )13	Yield coefficient for production of C_3 from C_1 mgC_2/mgC_1
177			YBW13	Water column biodegradation
179			YBS13	Benthic biodegradation
247			YHOH13	Alkaline hydrolysis
249			YHN13	Neutral hydrolysis
251			YHH13	Acid hydrolysis
282			YOX13	Oxidation
567			YF13	Photolysis
597			YE13	Extra reaction

TABLE 25 YIELD CONSTANTS FOR CHEMICAL 2 REACTIONS

Constant Number				
C_1	C_2	C_3	Variable	Definition
			Y( )21	Yield coefficient for production of C_1 from C_2, mgC_2/mgC_1
	776		YBW21	Water column biodegradation
	778		YBS21	Benthic biodegradation
	846		YHOH21	Alkaline hydrolysis
	848		YHN21	Neutral hydrolysis
	850		YHH21	Acid hydrolysis
	881		YOX21	Oxidation
	1166		YF21	Photolysis
	1196		YE21	Extra reaction
			Y( )23	Yield coefficient for production of C_3 from C_2, mgC_3/mgC_2
	777		YBW23	Water column biodegradation
	779		YBS23	Benthic biodegradation
	847		YHOH23	Alkaline hydrolysis
	849		YHN23	Neutral hydrolysis
	851		YHH23	Acid hydrolysis
	882		YOX23	Oxidation
	1167		YF23	Photolysis
	1197		YE23	Extra reaction

TABLE 26 YIELD CONSTANTS FOR CHEMICAL 3 REACTIONS

Constant Number				
C_1	C_2	C_3	Variable	Definition
			Y( )31	Yield coefficient for production of C_1 from C_3, mgC_1/mgC_2
		1376	YBW31	Water column biodegradation
		1378	YBS31	Benthic biodegradation
		1446	YHOH31	Alkaline hydrolysis
		1448	YHN31	Neutral hydrolysis
		1450	YHH31	Acid hydrolysis
		1481	YOX31	Oxidation
		1766	YF31	Photolysis
		1796	YE31	Extra reaction
			Y( )32	Yield coefficient for production of C_2 from C_3, mgC_2/mgC_3
		1377	YBW32	Water column biodegradation
		1379	YBS32	Benthic biodegradation
		1447	YHOH32	Alkaline hydrolysis
		1449	YHN32	Neutral hydrolysis
		1451	YHH32	Acid hydrolysis
		1482	YOX32	Oxidation
		1767	YF32	Photolysis
		1797	YE32	Extra reaction

CHAPTER 10

DATA GROUP I   KINETIC TIME FUNCTIONS

The definition of the kinetic time functions will vary depending upon the structure and the kinetics of the systems comprising each model The input format, however, is constant Time functions are input as piecewise linear functions

10 1 RECORD FORMATS

Record 1--Number of Time Functions (I10, 70X)

NFUNC = number of time functions required by the model If no time functions are to be input, set NFUNC equal to zero and go to Data Group J (I10)

TITLE = name of data group (70X)

Records 2-3 are input as a group NFUNC times

Record 2--Time Function Descriptions (A5, 2I5)

ANAME(ISC) = an optional one to five alphanumeric character descriptive name for the time function I (A5)

NOBRK(ISC) = number of breaks used to describe the time function I (I5)

ISC = number identifying the time function these numbers are set by the model developer (I5)

Record 3--Time Functions (4(2F10 0))

VALT(K) = value of time function ISC at time T(K) (F10 0)

T(K) = time in days If the length of the simulation exceeds T(NOBRK), the time function will repeat itself, starting at T(1), i e , the approximation is assumed to be periodic, with period equal to T(NOBRK) (F10 0)

Record 3 is repeated NOBRK(ISC)/4 times

Record 1 in entered once in Data Group I Records 2 and 3, as a set, are repeated NFUNC times Within each NFUNC set, Record 2 is input once and Record 3 uses as many 80-space lines as needed to input NOBRK entries Four entries (four VALK(K)-T(pairs) will fit on each 80-space line

10 2 THE EUTROPHICATION MODEL

Listed below are the 22 time functions available for eutrophication Only TEMP(1) is required for Level 1 and 2 analyses For Level 3 analyses, TFNH4, VELN(1), and WIND may be added (WIND is needed only for calculating reaeration in non-flowing water bodies such as lakes) For analyses at Level 4 and above, ITOT, F, KE, and TFPO4 should be used For resolutio of spatial variability in temperature, light extinction, and water velocity the four TEMP functions, the five KE functions, and the four VELN functions may be used

Many of the time functions operate in conjuction with a parameter "pointer in Data Group G The parameter value specifies which of several time functions for temperature, light extinction or water velocity are to be associated with each segment Time functions 1-4 are the four temperature functions available for parameter TMPFN Time functions 8-12 are the five extinction coefficient functions for parameter KEFN Functions 15-18 are the four water velocity options for VELFN

ISC	ANAME	Defininion and Units
1	TEMP(1)	Time-variable temperature function 1 TEMP(K) can be either a normalized function or an actual temperature in 蚓, depending upon the definition of the parameter multiplier TMPSG(ISEG)
2	TEMP(2)	Time-variable temperature function 2, unitless or 蚓
3	TEMP(3)	Time-variable temperature function 3, unitless or 蚓
4	TEMP(4)	Time-variable temperature function 4 unitless or 蚓
5	ITOT	Total daily solar radiation, langleys
6	F	Fraction of day with sufficient light for growth, days
7	WIND	Wind velocity, m/sec

8	KE(1)	Time-variable extinction coefficient function 1 This can be either a normalized function or an actual extinction coefficient in m^{1}, depending upon the definition of the parameter multiplier KESG(ISEG) 0 / ~ 5
9	KE(2)	Time-variable extinction coefficient function 2, unitless or m^{1}
10	KE(3)	Time-variable extinction coefficient function 3, unitless or m^{1}
11	KE(4)	Time-variable extinction coefficient function 4, unitless or m^{1}
12	KE(5)	Time-variable extinction coefficient function 5, unitless or m^{1}
13	TFNH4	Normalized ammonium flux from bed, unitless
14	TFPO4	Normalized phosphate flux from bed, unitless
15	VELN(1)	Time variable velocity function 1, m/sec This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C
16	VELN(2)	Time variable velocity function 2, m/sec
17	VELN(3)	Time variable velocity function 3, m/sec
18	VELN(4)	Time variable velocity function 4, m/sec
19	ZOO	Herbivorous zooplankton population, mgC/L
20	SALFN	Time variable salinity function mg/l This function gets multiplied by the segment specific salinity multiplier entered in the parameter sector
21	AIRTMP	Time variable ambient air temperature, °C This provides air temperature data for the wind driven reaeration algorithms and is required
22	XICEVR	This is the time variable ice cover function, % This provides the percentage of water surface area available for reaeration Note that 100% (entered as 1.0) indicates all surface area is available for reaeration

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10 3 THE TOXIC CHEMICAL MODEL

Listed below are the 17 time functions available in TOXI4 The parameters and time functions interact in such away to allow the user segment specific control of environmental data For more details see the parameter input section

Two of the time functions operate in conjuction with a parameter pointer" in Data Group G The parameter value specifies which of four time functions for temperature or water velocity are to be associated with each segment Time functions 1-4 are the four temperature functions available for parameter TMPFN Time functions 5-8 are the four water velocity options for VELFN

ISC	ANAME	VALT(ISC)
1	TEMPN(1)	Time-variable temperature function 1 TEMPN(K) can be either a normalized function or an actual temperature in 蚓, depending upon the definition of the parameter multiplier TEMP(ISEG)
2	TEMPN(2)	Time variable temperature function 2, unitless or 蚓
3	TEMPN(3)	Time variable temperature 3, unitless or 蚓
4	TEMPN(4)	Time variable temperature 4 unitless or 蚓
5	VELN(1)	Time variable velocity function 1, m/sec This velocity is added to the net velocity VELOCG(ISEG) parameters read in Data Group C
6	VELN(2)	Time variable velocity function 2 m/sec This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C
7	VELN(3)	Time variable velocity function 3 m/sec This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C
8	VELN(4)	Time variable velocity function 4, m/sec This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C
9	WINDN	Time variable wind function, m/sec This time function is multiplied by the segment specific

		wind multiplier WVEL entered in the parameter section
10	PHNW	Time variable ph function This time function is multiplied by the segment specific ph multiplier ph enter in the parameter section
11	PHNS	Normalized benthic pH function, dimensionless This is multiplied by the segment pH multiplier PH(ISEG) for benthic segments
12	REARN	Time variable reaeration coefficient, per day This variable is multiplied by the segment specific variable REAR entered in the parameter section
13	AIRTMPN	Air temperature, C Used for calculating reaeration rate
14	CHLN	Phytoplankton chlorophyll concentration mg/l This variable is multiplied by the segment specific variable CHPHL entered in the parameter section
15	PHTON	Normalized light intensity, dimensionless This is used for photolysis option 2 to adjust the measured rate constant under controlled light intensity to a predicted rate constant under ambient light intensity
16	BACNW	Time variable bacteria concentration in the water column, mg/l This is multiplied by the segment specific multiplier BAC entered in the parameter section
17	BACNS	Normalized benthic bacteria function dimensionless This is multiplied by the segment bacteria multiplier BAC(ISEG) for benthic segments

For kinetics levels 1 and 2 no time functions need be specified For kinetics level 3 time functions for each relevant process may be specified TEMPN can affect all reactions Volatilization option 1 uses REARN Volatilization options 4 and 5 use WINDN and AIRTMPN Volatilization options 2 and 3 use either VELN or REARN Photolysis option 1 uses CHLN photolysis option 2 requires PHTON Hydrolysis and ionization use PHNW and PHNS Biodegradation uses BACNW and BACNS Functions not specified default to 1 0

CHAPTER 11

DATA GROUP J INITIAL CONDITIONS

11 1 RECORD FORMATS

The initial conditions are the segment concentrations and densities for the state variables at time zero (the start of the simulation)

Records 1-2 are input as a group NOSYS times

<u>Record 1--System Information (A40, I5, F5.0, F10.0, 20X)</u>

CHEML = chemical or system name (A40)

IFIELD = solids field (3, 4, or 5) that transports this system in its pure or sorbed form (I5)

DSED = density of system, 0 0 for chemical 0 5-2 5 for solids, kg/L (F5 0)

CMAX = maximum concentration allowed mg/L (F10 0)

TITLE = name of data group (20X)

<u>Record 2--Initial Conditions (3(A5, 2F10.0))</u>

ANAME(K) = an optional one to five alphanumeric character descriptive name or number identifying segment K (A5)

C(ISYS,K) = initial concentration in segment K of system ISYS in the appropriate units, mg/L (F10 0)

DISSF = dissolved fraction of chemical in segment K (F10 0)

Record 2 is repeated NOSEG/3 times

Records 1 and 2 are a set and will be repeated NOSYS times Within each NOSYS set Record 2 will use as many 80-space lines as needed to input NOSEG entries Three entries (ANAME-C-DISSF) will fit on one line <u>After NOSEG entries have been entered in a NOSYS set, begin the next NOSYS set on the following line</u> If ICFL = 2 in Data Group A initial conditions are read from the restart file (* RST where * is the input data set name) and Data Group J should not be included in the input data set

11 2 THE EUTROPHICATION MODEL

Data Group J is input as a unit 8 times, once for each system In record 1, solids transport fields must be specified for the particulate fraction of each system In EUTRO4, solids field 3 is equated to particulate organic matter, solids field 4 is phytoplankton, and solids field 5 is inorganic sediment The following specifications, then, are recommended for systems 1 through 8

IFIELD(1) = 3 (solids field 1)

IFIELD(2) = 5 (solids field 3)

IFIELD(3) = 5 (solids field 3)

IFIELD(4) = 4 (solids field 2)

IFIELD(5) = 3 (solids field 1)

IFIELD(6) = 5 (solids field 3)

IFIELD(7) = 3 (solids field 1)

IFIELD(8) = 3 (solids field 1)

The density of each solid field must also be specified in record 1 This property is not used in EUTRO4 The user may enter 1 0 for the density of each system

The dissolved fraction of each system in each segment must be specified in record 2 The user should take care to specify the dissolved fractions for dissolved oxygen (system 6) of 1 0 and the dissolved fractions for phytoplankton (system 4) of 0 0

11 3 THE TOXIC CHEMICAL MODEL

Data Group J is input as a unit NOSYS times once for each system In record 1, solids transport fields must be specified for each solid (i e - variables 2 3 and 4) While solids transport fields are also specified for each chemical (variables 1, 5, and 6), the values are nominal TOXI4 will calculate the actual transport of the sorbed chemical fractions using internal partitioning relationships

In Record 2 the dissolved fraction of each system in each segment must be specified These values should be 1 0 for each solid variable (2, 3, and 4) Dissolved fraction values for each chemical are nominal TOXI4 will calculate the actual dissolved fractions using internal partitioning relationships

CHAPTER 12

WASP5 OUTPUT

12 1 GENERAL CONSIDERATIONS

WASP5 simulations produce several files that may be examined by the user These files use the file name of the input data set with a unique extension The most important of these are the simulation result files * TDF (TOXI4) and * EDF (EUTRO4), which contain all kinetic display variables for each segment at each print interval throughout the simulation These display variables include concentrations, certain calculated variables, and some rates Available display variables for EUTRO4 and TOXI4 are summarized in the eutrophication and toxics user manual sections

The simulation results files can be processed with the post processing programs available with the WISP package or the W4DSPLY program which is provided with the mainframe version The program will prompt the user for information

Other files created by a WASP simulation include * OUT, * TRN, * MSB, and * RST (where * is the name of the input data set) The OUT file contains a record of the input data plus any simulation error messages that may have been generated The TRN file contains a set of transport associated variables for each segment at each print interval throughout the simulation These variables include the time step (day) calculated maximum time steps (day), segment volumes (m^3), segment flows (m^3/sec), flow changes (m^3/sec), time constants for segment flow (day^{1}), segment exchange flows (m^3/sec) the time constant for segment exchanges (day^{1}), the segment dispersion coefficient (m^3/sec), and the numerical dispersion coefficient (m^2/sec) The MSB file contains a mass balance record for one designated system in the model network as a whole (in kg) For each print interval, this file records the accumulated mass in from advection dispersion and loading the accumulated mass out through advection, dispersion, burial (or volatilization and kinetic transformation, the total resident mass and the residual (unaccounted for) mass

The RST file contains a snapshot of volumes and concentrations of each system in each segment at the conclusion of the simulation This file can be read by WASP5 to continue a series of simulations

12 2 THE EUTROPHICATION MODEL

The standard WASP5 output files were summarized above EUTRO4 stores in the DMP file 36 kinetic display variables These ~~variables are listed below~~ To examine these variables in tabular form, the user may run WASP5 postprocessor

EUTRO4 KINETIC DISPLAY VARIABLES

Number	Definition
1	Segment Depth (m)
2	Segment Temperature (蚓)
3	Wind (m/sec)
4	Water Velocity (m/sec)
5	Dissolved Oxygen (mg/l)
6	DO Minimum (mg/l)
7	DO Maximum (mg/l)
8	DO Saturation (mg/l)
9	Percent Saturation
10	Reaeration Rate (day-1)
11	Wind Driven KA (day-1)
12	Hydraulic KA (day-1)
13	Sediment O2 Demand (g/m2/day)
14	CBOD (mg/l)
15	BOD5 (mg/l)
16	Ultimate BOD (mg/l)
17	Temperature Corrected KBOD (mg/l)
18	Phyto Biomass (carbon) (mg/l)
19	Total Chl-a (痢/l)
20	Growth rate (day-1)
21	Death Rate (day-1)
22	Algae DO Production (mg/l/day)
23	Algae DO Consumption (mg/l/day)
24	Carbon to Chl-a Ratio (mg/mg)
25	Light Limit for Algae

EUTRO4 KINETIC DISPLAY VARIABLES

Number	Definition
26	Nutrient LImit for Algae
27	P Limit
28	N Limit
29	Average Light at Surface (langleys/day)
30	Saturating Light (langleys/day)
31	Light at Top of Segment (langleys/day)
32	Light at Bottom Segment (langleys/day)
33	Ammonia N (mg/l)
34	Nitrate N (mg/l)
35	Organic N (on Living) (mg/l)
36	Total Organic N (mg/l)
37	Total Nitrogen (mg/l)
38	Available Inorganic P (mg/l)
39	Total Inorganic P (mg/l)
40	Total Organic P (mg/l)
41	Organic P (non-living) (mg/l)
42	Preference NH3-NO3

12 3 THE TOXIC CHEMICAL MODEL

The standard WASP5 output files were summarized in Section 2 3 TOXI4 stores in the DMP file 18 30 or 42 kinetic display variables depending on whether 1, 2 or 3 chemicals were simulated These variables are defined below To examine these variables in tabular form, the user may run W4DSPLY as explained in Section 2 3

TOXI4 DISPLAY VARIABLES

Constant Number				
C_1	C_2	C_3	Variable	Definition
1			TOTSOSL	Total solids concentration, mg/L
2			SOLID 1	Solids type 1 concentration, mg/L
3			SOLID 2	Solids type 2 concentration, mg/L
4			SOLID 3	Solids type 3 concentration, mg/L
5			STEMP	Segment temperature 蚓
6			ITYPE	Segment type (1, 2, 3, or 4)
7	19	31	TOTCHEM	Total chemical concentration (1, 2, or 3) 痢/L
8	20	32	TOTDIS	Dissolved chemical concentration, 痢/L
9	21	33	TOTDOC	DOC-sorbed chemical concentration, 痢/L
10	22	34	TOTPAR	Total sorbed chemical concentration, 痢/L
11	23	35	TOTPAP1	Total sorbed chemical concentration, 痢/kg
12	24	36	TOTION	Total ionic chemical concentration, 痢/L
13	25	37	KB10	Biodegradation rate constant, day^{1}
14	26	38	KHYD	Total hydrolysis rate constant, day^{1}
15	27	39	KFOT	Photolysis rate constant, day^{1}
16	28	40	KVOL	Volatilization rate constant day^{1}
17	29	41	KOX	Oxidation rate constant day^{1}
18	30	42	KEXT	Extra rate constant, day^{1}

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THE ENHANCED STREAM WATER QUALITY MODELS QUAL2E AND QUAL2E-UNCAS DOCUMENTATION AND USER MANUAL

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DISCLAIMER

FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient management tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact and control of environmental contaminants, the Assessment Branch develops management or engineering tools to help pollution control officials achieve water quality goals.

The stream water quality model QUAL2E is widely used for waste load allocations, discharge permit determinations, and other conventional pollutant evaluations in the United States. Since the introduction of QUAL-II in 1970, several different versions of the model have evolved. This manual presents the most recent modifications in the form of enhanced state-of-the-art models called QUAL2E and QUAL2E-UNCAS. Both models have been developed over the past three years through cooperative agreements between the National Council for Air and Stream Improvement (NCASI), the Department of Civil Engineering at Tufts University, and EPA. Distribution and maintenance of the QUAL2E and QUAL2E-UNCAS computer programs, and training and assistance to model users, will be provided by EPA's Center for Water Quality Modeling at this Laboratory.

Rosemarie C. Russo, Ph.D.
Director
Environmental Research Laboratory
Athens, Georgia

ABSTRACT

This manual is a major revision to the original QUAL2E Program Documentation (EPA/600/3-85/065) released in 1985. It includes a description of the recent modifications and improvements to the widely used water quality models QUAL-II and QUAL2E. The enhancements to QUAL-II that led to QUAL2E incorporated improvements in eight areas: (1) algal, nitrogen, phosphorus, and dissolved oxygen interactions, (2) algal growth rate, (3) temperature, (4) dissolved oxygen, (5) arbitrary non-conservative constituents, (6) hydraulics, (7) downstream boundary concentrations, and (8) input/output modifications. These are fully documented in this manual. The enhancements to QUAL2E, described for the first time in this report, include (1) an extensive capability for uncertainty analysis with the model QUAL2E-UNCAS, (2) an option for reach-variable climatology input for steady state temperature simulation, and (3) an option for plotting observed dissolved oxygen data on the line printer plots of predicted dissolved oxygen concentrations.

QUAL2E, which can be operated either as a steady-state or as a dynamic model, is intended for use as a water quality planning tool. The model can be used, for example, to study the impact of waste loads on instream water quality or to identify the magnitude and quality characteristics of nonpoint waste loads as part of a field sampling program. The user also can model effects of diurnal variations in meteorological data on water quality (primarily dissolved oxygen and temperature) or examine diurnal dissolved oxygen variations caused by algal growth and respiration.

QUAL2E-UNCAS is an enhancement to QUAL2E that allows the user to perform uncertainty analysis. Three uncertainty options are available: sensitivity analysis, first order error analysis, and monte carlo simulation. With this capability, the user can assess the effect of model sensitivities and of uncertain input data on model forecasts.

This report was submitted in partial fulfillment of Cooperative Agreement No. 811883 by Tufts University under the partial sponsorship of the U.S. Environmental Protection Agency. This report covers a period from June 1985 to January 1987, and work was completed as of January 1987.

CONTENTS

CONTENTS (Cont'd)

CONTENTS (Cont'd)

LIST OF FIGURES

LIST OF TABLES

ACKNOWLEDGMENT

Over the years, many investigators have contributed to the development of what has become QUAL2E. The foundation upon which the model has been built was laid by the Texas Water Development Board in the late 1960s in the QUAL-I model. Many versions of the model emerged in the 1970s. The lineage of QUAL2E can be traced to work done for the Southeast Michigan Council of Governments (SEMCOG) by Water Resources Engineers, Inc. (now Camp, Dresser, McKee, Inc.). QUAL-II/SEMCOG was chosen for distribution by the Center for Water Quality Modeling (CWQM) in the late 1970s and began to receive wide use in water quality modeling and wasteload allocation programs.

QUAL-II/SEMCOG was thoroughly reviewed, tested, and documented by the National Council of the Paper Industry for Air and Stream Improvement, Inc. (NCASI), as discussed in NCASI Technical Bulletin No. 391. Changes arising from this review were incorporated in a model called QUAL-II/NCASI, which was adopted for distribution by the Center for Water Quality Modeling. Because of a mutual interest in the program, CWQM partially sponsored an NCASI review of other versions of the QUAL-II computer program and incorporated useful features of these versions in the program called QUAL2E.

Appendix A of this documentation report, the QUAL2E users manual, is modeled after NCASI Technical Bulletin No. 457, "Modifications to the QUAL-2 Water Quality Model and User Manual for QUAL2E Version 2.2." We express our appreciation to NCASI for permission to use and modify this material in this report.

The QUAL2E program also has been made available for IBM PC-compatible microcomputer. The microcomputer installation of this program was performed by Mr. Bruce Bartell and Mr. David Disney of Computer Sciences Corporation, Inc. and was made possible through the support of Mr. King Boynton of the U.S. EPA's Office of Water and through an agreement with the US-Spain Joint Committee for Scientific and Technical Cooperation.

The current release of the program incorporates modifications to the 1985 release to accommodate large elevation differences along a river funded through an agreement with the US-Spain Joint Committee for Scientific and Technical Cooperation. The major extension to the program documented herein, the uncertainty analysis capability, was begun by the first author while on a sabbatical year (1984) from Tufts University at the Athens Environmental Research Laboratory and completed on his return to academic work.

1 INTRODUCTION

QUAL2E is a comprehensive and versatile stream water quality model It can simulate up to 15 water quality constituents in any combination desired by the user Constituents which can be simulated are

1. Dissolved Oxygen
2. Biochemical Oxygen Demand
3. Temperature
4. Algae as Chlorophyll _a_
5. Organic Nitrogen as N
6. Ammonia as N
7. Nitrite as N
8. Nitrate as N
9. Organic Phosphorus as P
10. Dissolved Phosphorus as P
11. Coliforms
12. Arbitrary Nonconservative Constituent
13. Three Conservative Constituents

The model is applicable to dendritic streams that are well mixed It assumes that the major transport mechanisms advection and dispersion, are significant only along the main direction of flow (longitudinal axis of the stream or canal) It allows for multiple waste discharges, withdrawals, tributary flows, and incremental inflow and outflow It also has the capability to compute required dilution flows for flow augmentation to meet any prespecified dissolved oxygen level

Hydraulically, QUAL2E is limited to the simulation of time periods during which both the stream flow in river basins and input waste loads are essentially constant QUAL2E can operate either as a steady-state or as a dynamic model, making it a very helpful water quality planning tool When operated as a steady-state model, it can be used to study the impact of waste loads (magnitude, quality and location) on instream water quality and also can be used in conjunction with a field sampling program to identify the magnitude and quality characteristics of nonpoint source waste loads. By operating the model dynamically, the user can study the effects of diurnal variations in meteorological data on water quality (primarily dissolved oxygen and temperature) and also can study diurnal dissolved oxygen variations due to algal growth and respiration. However, the effects of dynamic forcing functions, such as headwater flows or point loads, cannot be modeled in QUAL2E.

QUAL2E-UNCAS is a recent enhancement to QUAL2E which allows the modeler to perform uncertainty analysis on the steady state water quality simulations. Three uncertainty options are available: sensitivity analysis, first order error analysis, and monte carlo simulations. With this capability, the user can assess the effect of model sensitivities and of uncertain input data on model forecasts. Quantifications of the uncertainty in model forecasts will allow assessment of the risk (probability) of a water quality variable being above or below an acceptable level. The uncertainty methodologies provide the means whereby variance estimates and uncertainty prediction can become as much a part of water quality modeling as estimating expected values is today. An evaluation of the input factors that contribute most to the level of uncertainty will lead modelers in the direction of most efficient data gathering and research. In this manner the modeler can assess the risk of imprecise forecasts and recommend measures for reducing the magnitude of that imprecision.

1.1 QUAL2E DEVELOPMENT

1.1.1 Current Release

The current release of QUAL2E (Version 3.0) was developed under a cooperative agreement between Tufts University, Department of Civil Engineering and the EPA Center for Water Quality Modeling (CWQM), Environmental Research Laboratory, Athens, GA. It includes modifications to prior releases of QUAL2E (Version 2.2, Brown and Barnwell, 1985) as well as an extensive capability for uncertainty analysis (UNCAS) of its steady state simulation output. This release of QUAL2E and its companion program for uncertainty analysis, QUAL2E-UNCAS, is intended to supercede all prior releases of QUAL2E and QUAL-II.

1.1.2 History

The original QUAL-II model was an extension of the stream water quality model QUAL-I developed by F. D. Masch and Associates and the Texas Water Development Board (1971) and the Texas Water Development Board (1970). In 1972, Water Resources Engineers, Inc. (WRE) under contract to the U.S. Environmental Protection Agency, modified and extended QUAL-I to produce the first version of QUAL-II. Over the next 3 years, several different versions of the model evolved in response to specific user needs. In March 1976, the Southeast Michigan Council of Governments (SEMCOG) contracted with WRE to make further modifications and to combine the best features of the existing versions of QUAL-II into a single model. The significant modifications made in the SEMCOG version by WRE (Roesner et al., 1981a and b) were:

- Option of English or metric units on input data
- Option for English or metric output--choice is independent of input units
- Option to specify channel hydraulic properties in terms of trapezoidal channels or stage-discharge and velocity-discharge curves
- Option to use Tsivoglou's computational method for stream reaeration
- Improvement in output display routines
- Improvement in steady-state temperature computation routines

The SEMCOG version of QUAL-II was later reviewed, documented, and revised (NCASI, 1982). The revised SEMCOG version has since been maintained and supported by the EPA Center for Water Quality Modeling (CWQM). In 1983, EPA, through the CWQM, contracted with NCASI to continue the process of modifying QUAL-II to reflect state-of-the-art water quality modeling. Extensive use of QUAL-II/SEMCOG had uncovered difficulties that required corrections in the algal-nutrient-light interactions. In addition, a number of modifications to the program input and output had been suggested by users. The enhanced QUAL-II model was renamed QUAL2E (Brown and Barnwell, 1985) and incorporated improvements in eight areas. These enhancements are fully documented in this report and summarized as follows:

1. Algal, nitrogen, phosphorus, dissolved oxygen interactions
    - Organic nitrogen state variable
    - Organic phosphorus state variable
    - Nitrification inhibition at low DO
    - Algal preference factor for NH_3
2. Algal growth rate
    - Growth rate dependent upon both NH_3 and NO_3 concentrations
    - Algal self-shading
    - Three light functions for growth rate attenuation
    - Three growth rate attenuation options
    - Four diurnal averaging options for light
3. Temperature
    - Link to algal growth via solar radiation
    - Default temperature correction factors
4. Dissolved Oxygen (DO)
    - 6th Edition on Standard Methods DO saturation function

- Traditional SOD units (g/m^2-day or g/ft^2-day)
- Dam reaeration option

5. Arbitrary non-conservative constituent

   - First order decay
   - Removal (settling) term
   - Benthal source term

6. Hydraulics

   - Input factor for longitudinal dispersion
   - Test for negative flow (i.e., withdrawal greater than flow)
   - Capability for incremental outflow along reach

7. Downstream boundary

   - Option for specifying downstream boundary water quality constituent concentrations

8. Input/output modifications

   - Detailed summary of hydraulic calculations

   - New coding forms

   - Local climatological data echo printed

   - Enhanced steady-state convergence

   - Five part final summary including components of DO deficit and plot of DO and BOD

1.1.3 Enhancements to QUAL2E

Since the first release of QUAL2E in 1985, enhancements to the model have continued. The modifications, listed below, are designed to improve the computational efficiency of the code, as well as to assist the user in model calibration and verification. The reach variable climatology modifications were added in response to applications of QUAL2E to the river network in Madrid, Spain. In that system, large changes in elevation presented difficulties in calibrating QUAL2E for temperature and dissolved oxygen. The major addition to the current release of QUAL2E is the uncertainty analysis capability. Inclusion of this feature resulted from a project which investigated various methodologies for incorporating uncertainty analysis as an integral part of the water quality modeling process. The QUAL2E model was chosen for this application because it is a general purpose computer code, widely used by consultants and state regulatory agencies in waste load allocation and other planning activities.

Enhancements to QUAL2E in the current release include:

1 Option for reach variable climatology input for steady state temperature simulation

2 Option for including observed dissolved oxygen data on the line printer plots of predicted dissolved oxygen concentrations

3 Changing the steady state convergence criterion for algal, nitrification, and dissolved oxygen simulations from an absolute error to a relative error

4 Updating the formulation for estimating reaeration effects of water flowing over a dam

Capabilities of the uncertainty analysis model, QUAL2E-UNCAS, include the following

1 *Sensitivity analysis*--with an option for factorially designed combinations of input variable perturbations

2 *First order error analysis*--with output consisting of a normalized sensitivity coefficient matrix, and a components of variance matrix

3 *Monte carlo simulation*--with summary statistics and frequency distributions of the output variables

1 1 4 *Information Sources*

Major sources of information for this revised documentation are

1 Roesner, L A , Giguere, P R and Evenson, D E *Computer Program Documentation for Stream Quality Modeling (QUAL-II)* U S Environmental Protection Athens, GA EPA-600/9-81-014, February 1981

2 JRB Associates *Users Manual for Vermont QUAL-II Model* Prepared for U S Environmental Protection Agency, Washington, DC June 1983

3 National Council for Air and Stream Improvement *A Review of the Mathematical Water Quality Model QUAL-II and Guidance for its Use*, NCASI, New York, NY, Technical Bulletin No 391, December 1982

4 Brown, L C and T O Barnwell, Jr , *Computer Program Documentation for the Enhanced Stream Water Quality Model QUAL2E*, U S Environmental Protection Agency, Environmental Research Laboratory, Athens, GA EPA/600-3-85/065, August 1985

This documentation of QUAL2E updates the report distributed with the prior version of the model (Brown and Barnwell, 1985) and consolidates material from these and other sources into a single volume The basic theory and mechanics behind the development of QUAL2E are described in this volume. The two appendices contain user manuals for QUAL2E and QUAL2E-UNCAS and provide a detailed description of input data requirements, as well as sample input coding forms. This report, a copy of the QUAL2E and QUAL2E-UNCAS computer code, and sample input/output data files are available from the Center for Water Quality Modeling, U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA 30613.

1.1.5 Organization of this Report

The general program structure, specifications, and limitations of QUAL2E are discussed in the remainder of this chapter. Chapter 2 describes the conceptual and functional representation of QUAL2E as well as the hydraulic characteristics of the model. The mathematical basis of the water quality constituent formulations is presented in Chapter 3. Chapter 4 presents the framework for modeling temperature. With the exception of Section 4.8, it is extracted essentially verbatim from Roesner *et al.*, 1981. Chapter 5 describes the computational representation of the model and the numerical solution algorithm.

The uncertainty analysis capabilities of QUAL2E-UNCAS are documented in Chapter 6.

Appendix A contains a user manual complete with revised input coding forms for the current release (Version 3.0) of QUAL2E. Appendix B is the user manual for QUAL2E-UNCAS. Appendix C describes an example application of QUAL2E-UNCAS.

For the convenience of the majority of users, all of the units specifications are given in the English system of measurement. QUAL2E however will recognize either English or metric units.

1.2 QUAL2E COMPUTER MODEL

1.2.1 Prototype Representation

QUAL2E permits simulation of any branching, one-dimensional stream system. The first step in modeling a system is to subdivide the stream system into *reaches*, which are stretches of stream that have uniform hydraulic characteristics. Each reach is then divided into computational elements of equal length. Thus, all reaches must consist of an integer number of computational elements.

There are seven different types of computational elements:

1. Headwater element

2. Standard element

3. Element just upstream from a junction

4 Junction element

5 Last element in system

6 Input element

7 Withdrawal element

Headwater elements begin every tributary as well as the main river system, and as such, they must always be the first element in a headwater reach. A standard element is one that does not qualify as one of the remaining six element types. Because incremental flow is permitted in all element types, the only input permitted in a standard element is incremental flow. A type 3 element is used to designate an element on the main stem just upstream of a junction. A junction element (type 4) has a simulated tributary entering it. Element type 5 identifies the last computational element in the river system; there should be only one type 5 element. Element types 6 and 7 represent inputs (waste loads and unsimulated tributaries) and water withdrawals, respectively. River reaches, which are aggregates of computational elements, are the basis of most data input. Hydraulic data, reaction rate coefficients, initial conditions, and incremental flows data are constant for all computational elements within a reach.

2.2 Model Limitations

QUAL2E has been designed to be a relatively general program; however, certain dimensional limitations have been imposed during program development. These limitations are:

- Reaches: a maximum of 25
- Computational elements: no more than 20 per reach or a total of 250
- Headwater elements: a maximum of 7
- Junction elements: a maximum of 6
- Input and withdrawal elements: a maximum of 25

QUAL2E incorporates features of ANSI FORTRAN 77 that allow these limitations to be easily changed.

2.3 Model Structure and Subroutines

QUAL2E is structured as one main program supported by 51 different subroutines. Figure 2-1 illustrates the functional relationships between the main program and the subroutines. New state variables can be added or modifications to existing relationships can be made with a minimum of model restructuring through the simple addition of appropriate subroutines.

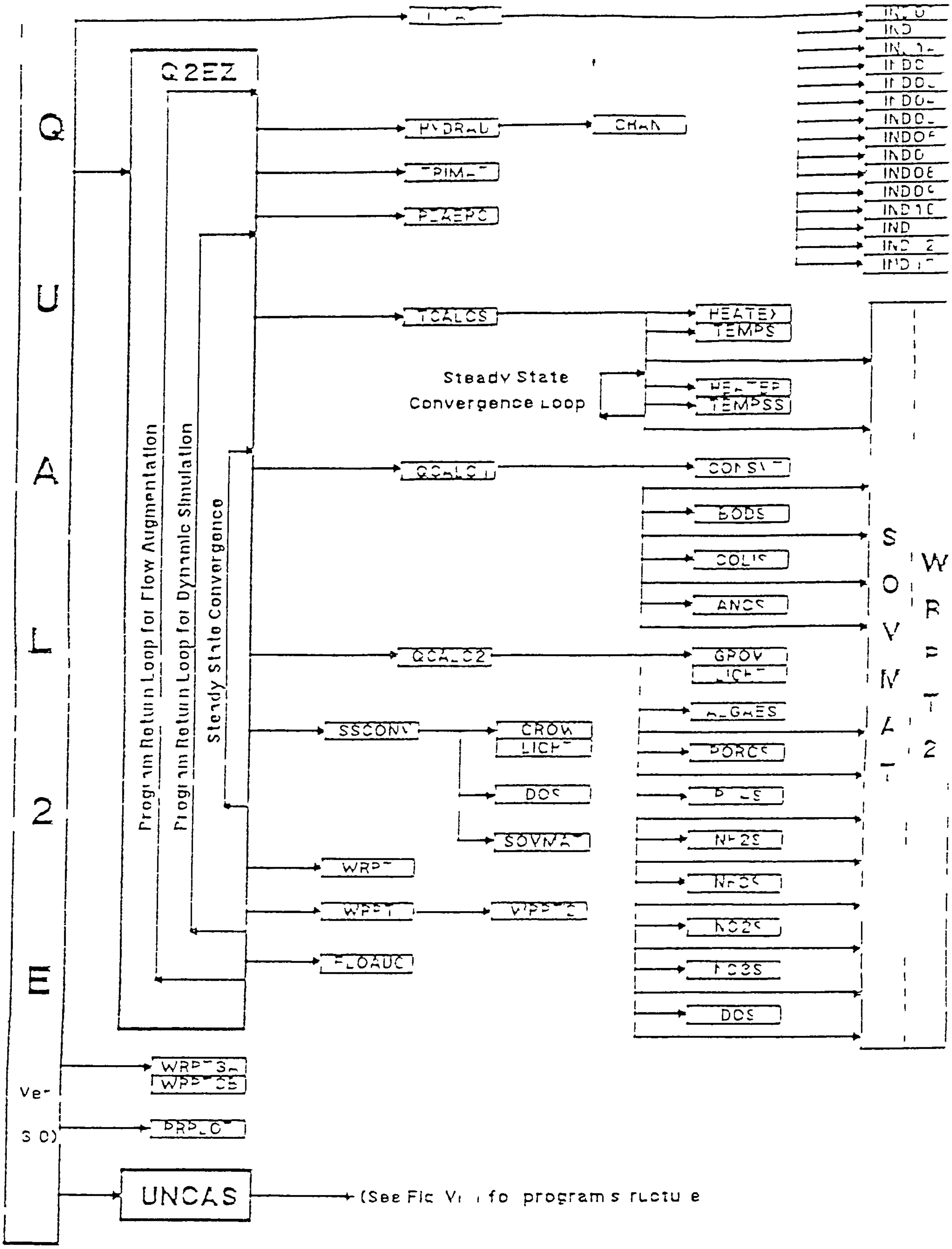

Figure I-1 General Structure of QUAL2E

The structural framework of QUAL2E has been modified from prior versions of QUAL-II. The large MAIN program and subroutine INDATA have been divided into smaller groups of subroutines, each with a more narrowly defined task. The new subroutines in QUAL2E include the algal light functions (GROW/LTCHT), the steady state algal output summary (WRPT1), the organic nitrogen and phosphorus state variables (NH2S, PORG), and the line printer plot routine (PRPLOT). This reorganization of QUAL2E into smaller programmatic units is the first step in adapting the model to micro and minicomputers that have limited memory.

QUAL2E Version 3.0 retains this modular program structure. QUAL2E may be obtained with or without the UNCAS capability. The program structure and subroutine descriptions for UNCAS are described in Chapter 6 of this report.

1.2.1 Program Language and Operating Requirements

QUAL2E is written in ANSI FORTRAN 77 and is compatible with mainframe and personal computer systems that support this language. QUAL2E typically requires 256K bytes of memory and uses a single system input device (cards or disk file) and the system's line printer (or disk file) as the output device.

If the system's normal FORTRAN input device unit is not unit 1 or the output unit is not unit 7, then the variables "NI" and "NO" in the main program (files Q2ECP0 or Q2UCP0) should be changed to reflect the system's I/O unit identifiers.

2 GENERAL MODEL FORMULATION

2.1 INTRODUCTION

The primary objective of any stream water quality model development is to produce a tool that has the capability for simulating the behavior of the hydrologic and water quality components of a stream system. The development of this tool to simulate prototype behavior by applying a mathematical model on a digital computer proceeds through three general phases (Water Resources Engineers, Inc., 1967).

1. Conceptual representation
2. Functional representation
3. Computational representation

Conceptual representation involves a graphic idealization of the prototype by description of the geometric properties that are to be modeled and by identification of boundary conditions and interrelationships between various parts of the prototype. Usually, this process entails dividing the prototype into discrete "elements" of a size compatible with the objectives that the model must serve, defining these elements according to some simple geometric rules, and designating the mode by which they are connected, either physically or functionally, as integral parts of the whole. A part of this conceptual structuring is the designation of those boundary conditions to be considered in the simulation.

Functional representation entails formulation of the physical features, processes, and boundary conditions into sets of algebraic equations. It involves precise definition of each variable and its relationship to all other parameters that characterize the model or its input-output relationships.

Computational representation is the process whereby the functional model is translated into the mathematical forms and computational procedures required for solution of the problem over the desired time and space continuum. It is concerned with development of a specific solution technique that can be accommodated by the computer and with codification of the technique in computer language.

In the remainder of this section the Conceptual Representation of QUAL2E will be described together with its general functional representation for mass transport, hydraulic characteristics, and longitudinal dispersion.

Chapter 3 will discuss specific constituent reactions and interactions. Chapter 4 will develop the functional representation of stream temperature as simulated in QUAL2E.

2.2 CONCEPTUAL REPRESENTATION

Figure II-1 shows a stream reach (n) that has been divided into a number of subreaches or computational elements, each of length Δx. For each of these computational elements, the hydrologic balance can be written in terms of flows into the upstream face of the element (Q_{i-1}), external sources or withdrawals (Qx_i), and the outflow (Q_i) through the downstream face of the element. Similarly, a materials balance for any constituent C can be written for the element. In the materials balance, we consider both transport ($Q \cdot C$) and dispersion ($A_x D_L \frac{\partial C}{\partial x}$) as the movers of mass along the stream axis. Mass can be added to or removed from the system via external sources and withdrawals $(QxCx)_i$ and added or removed via internal sources or sinks (S_i) such as benthic sources and biological transformation. Each computational element is considered to be completely mixed.

Thus, the stream can be conceptualized as a string of completely mixed reactors--computational elements--that are linked sequentially to one another via the mechanisms of transport and dispersion. Sequential groups of these reactors can be defined as reaches in which the computational elements have the same hydrogeometric properties--stream slope, channel cross section, roughness, etc.--and biological rate constants--BOD decay rate, benthic source rates, algae settling rates, etc.--so that the stream shown at the left of Figure II-2 can be conceptually represented by the grouping of reaches and computational elements shown on the right of Figure II-2.

2.3 FUNCTIONAL REPRESENTATION

2.3.1 Mass Transport Equation

The basic equation solved by QUAL2E is the one dimensional advection-dispersion mass transport equation, which is numerically integrated over space and time for each water quality constituent. This equation includes the effects of advection, dispersion, dilution, constituent reactions and interactions, and sources and sinks. For any constituent, C, this equation can be written as:

$$\frac{\partial M}{\partial t} = \frac{\partial\left(A_x D_L \frac{\partial C}{\partial x}\right)}{\partial x} dx - \frac{\partial\left(A_x \bar{u} C\right)}{\partial x} dx + \left(A_x\, dx\right) \frac{dC}{dt} + s \qquad \text{(II-1)}$$

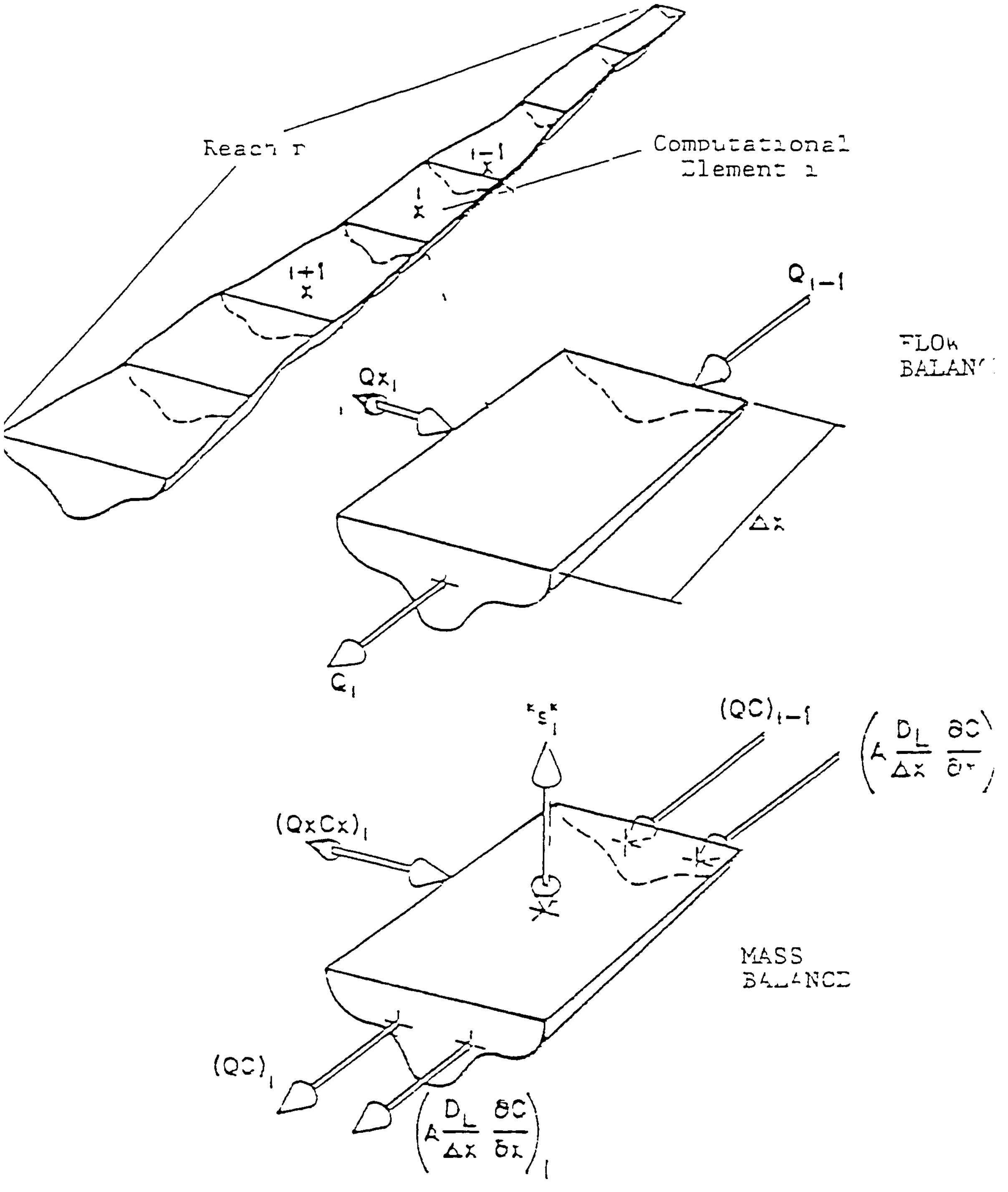

Figure II-1 Discretized Stream System

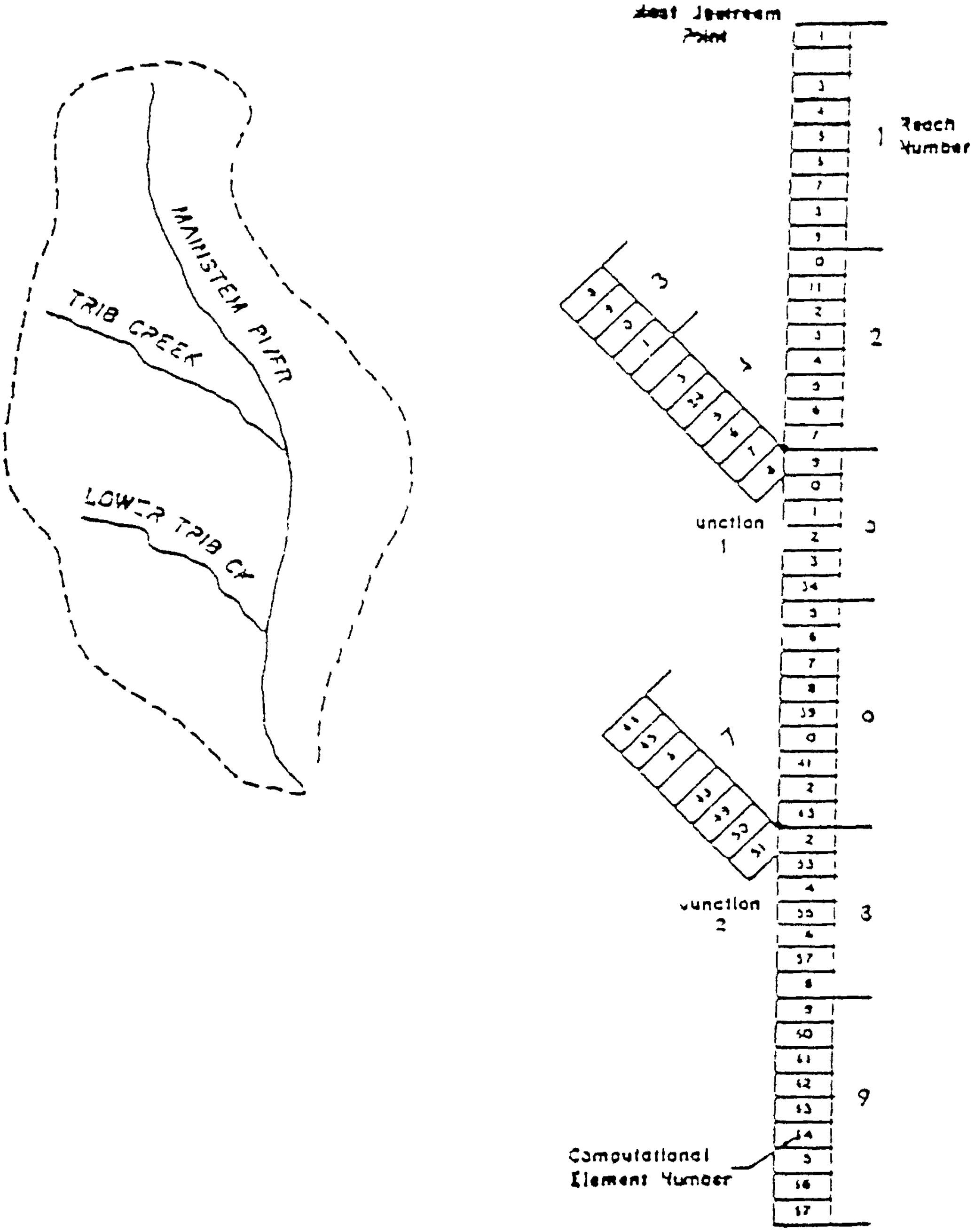

Figure -2 Stream Network of Computational Elements and Reaches

where

M = mass (M)

x = distance (L)

t = time (T)

C = concentration ($M\ L^{-3}$)

A_x = cross-sectional area (L^2)

D_L = dispersion coefficient ($L^2\ T^{-1}$)

$\overline{u}$ = mean velocity ($L\ T^{-1}$)

s = external source or sinks ($M\ T^{-1}$)

Because $M = VC$, we can write

$$\frac{\partial M}{\partial t} = \frac{\partial (VC)}{\partial t} = V \frac{\partial C}{\partial t} - C \frac{\partial V}{\partial t} \qquad \text{II-2a}$$

where

$V = A_x\ dx$ = incremental volume (L^3)

If we assume that the flow in the stream is steady, i e , $\partial Q/\partial t = 0$, then the term $\partial V/\partial t = 0$ and equation II-2a becomes

$$\frac{\partial M}{\partial t} = V \frac{\partial C}{\partial t} \qquad \text{II-2b}$$

Combining equations I - and -2b and rearranging,

$$\frac{\partial C}{\partial t} = \frac{\partial (A_x D_L \frac{\partial C}{\partial x})}{A_x\ \partial x} - \frac{\partial (A_x\ \overline{u}\ C)}{A_x\ \partial x} \quad \frac{dC}{dt} + \frac{s}{V} \qquad \text{II-3}$$

The terms on the right-hand side of the equation represent, respectively, dispersion, advection, constituent changes, external sources/sinks, and dilution The $\frac{dC}{dt}$ term refers only to constituent changes such as growth and decay, and should not be confused with the term $\frac{\partial C}{\partial t}$, the local concentration gradient The latter term includes the effect of constituent changes as well as dispersion, advection, sources/sinks, and dilutions

Under steady-state conditions, the local derivative becomes equal to zero, in other words

$$\frac{\partial C}{\partial t} = 0 \qquad \text{II-4}$$

Changes that occur to individual constituents or particles independent of advection, dispersion, and waste inputs are defined by the term

$$\frac{dC}{dt} = \text{individual constituents changes} \qquad \text{II-5}$$

These changes include the physical, chemical, and biological reactions and interactions that occur in the stream. Examples of these changes are reaeration, algal respiration and photosynthesis, and coliform die-off.

2.2 HYDRAULIC CHARACTERISTICS

QUAL2E assumes that the stream hydraulic regime is steady-state, i.e., $\partial Q/\partial t = 0$, therefore, the hydrologic balance for a computational element can be written simply as (see Figure [illegible])

$$\left(\frac{\partial Q}{\partial x}\right)_i = (Q_x)_i \qquad \text{II-6}$$

where $(Q_x)_i$ is the sum of the external inflows and/or withdrawals to that element.

2.2.1 Discharge Coefficients

Once equation II-6 has been solved for Q, the other hydraulic characteristics of the stream segments can be determined by equations of the form

$$\bar{u} = aQ^b \qquad \text{II-7}$$

$$A_x = Q/\bar{u} \qquad \text{II-8}$$

and

$$d = \alpha Q^\beta \qquad \text{II-9}$$

where a, b, α and β are empirical constants, and d is the stream depth. These constants usually can be determined from stage-discharge rating curves.

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where a, b, α and β are empirical constants, and d is the stream depth. These constants usually can be determined from stage-discharge rating curves.

Elder (1959) assumed that only the vertical velocity gradient was important in streamflow and developed an expression analogous to Taylor's expression

$$D_L = K d u^*$$ II-13

where d is the mean depth in feet of the stream. Elder used a value of 5.93 for K in this equation.

Other investigators have derived similar expressions for D_L and found it to be extremely sensitive to lateral velocity profiles. Elder's expression, however, seems adequate in one-dimensional situations where the channel is not too wide. For very wide channels, Fisher (1964) has shown that half-width rather than depth is the dominant scale and therefore is important to the definition of the longitudinal dispersion coefficient. Equations II-11 and II-13 can be written in terms of the Manning Equation and other variables characteristic of stream channels.

As an example, for steady-state open-channel flow

$$u^* = C\sqrt{RS_e}$$ II-14

where

C = Chezy's coefficient

R = the hydraulic radius

S_e = the slope of the energy grade line

Chezy's coefficient is given by

$$C = \frac{R^{1/6}}{n}$$ II-15

where n is the Manning roughness coefficient tabulated for different types of channels in Table I-

S_e, the slope of the energy gradient, is given by

$$S_e = \left(\frac{\overline{u}\, n}{1.486\, R^{2/3}}\right)^2$$ II-16

where $\overline{u}$ is the mean velocity. Substituting equations II-14, II-15 and II-16 into equation II-13 and letting R = d for a wide channel yields the expression

$$D_L = 3.32\, K\, n\, \overline{u}\, d^{5/6}$$ II-17

TABLE II-1

VALUES OF MANNING'S "n" ROUGHNESS COEFFICIENT

After Henderson (1966)

Artificial Channels	n
Glass, plastic, machined metal	0.010
Dressed timber, joints flush	0.011
Sawn timber, joints uneven	0.014
Cement plaster	0.011
Concrete, steel troweled	0.012
Concrete, timber forms, unfinished	0.014
Untreated gunite	0.015-0.017
Brickwork or dressed masonry	0.014
Rubble set in cement	0.017
Earth, smooth, no weeds	0.020
Earth, some stones, and weeds	0.025
Natural River Channels	**n**
Clean and straight	0.025-0.030
Winding with pools and shoals	0.033-0.040
Very weedy, winding and overgrown	0.075-0.150
Clean straight alluvial channels	$0.031\ d^{1/6}$ (d = D-75 size in ft = diameter that 75 percent of particles are smaller than)

where

D_L = longitudinal dispersion coefficient, ft^2/sec

K = dispersion constant (dimensionless)

n = Manning's roughness coefficient (dimensionless)

$\bar{U}$ = mean velocity, ft/sec

d = mean depth, ft

Typical values for dispersion coefficients, D_L, and values of the dispersion constant, K, cited by Fisher et al (1979), are given in Table II-2 Note that the dispersion constant, K, shown in this table is one to three orders of magnitude greater than that used by Elder

2 5 Flow Augmentation

When the DO concentration in a stream drops below some required target level, such as the state water quality standard for DO, it may be desirable to raise this DO concentration by augmenting the flow of the stream According to the originators of the flow augmentation routine in QUAL2E, Frank J Masch and Associates and the Texas Water Development Board (1971), the amount of flow necessary to bring the DO concentrations up to required standards cannot be calculated by an exact functional relationship A good approximation of the relationship is used in QUAL2E and has the following quadratic form

$$DO_R = DO_T - DO_{min} \qquad \text{II-18}$$

and

$$Q_R = Q_C\left[\frac{DO_R}{DO_T} - 0.5\left(\frac{DO_R}{DO_T}\right)^2\right] \qquad \text{II-19}$$

where,

DO_R = dissolved xoygen concentration required to meet target conditions, mg/L

DO_T = required target level of DO, mg/L

DO_{min} = minimum DO concentration (critical level) in the oxygen sag curve, mg/L

Q_R = amount of flow augmentation required, ft^3/sec

Q_C = flow at the critical point in the oxygen sag curve, ft^3/sec

TABLE II-2

EXPERIMENTAL MEASUREMENTS OF LONGITUDINAL DISPERSION IN OPEN CHANNELS

(After Table 5.3, Fisher et al., 1979)

Channel	Depth d (ft)	Width W (ft)	Mean Velocity $\overline{u}$ (ft/sec)	Shear Velocity u^* (ft/sec)	Dispersion Coefficient D_L (ft^2/sec)	Dispersi Constan k
Chicago Ship Channel	26.5	160	0.89	0.063	32	20
Sacramento River	13.1	--	1.74	0.17	161	74
River Derwent	0.82	--	1.25	0.46	50	131
South Platte River	1.5	--	2.17	0.23	174	510
Yuma Mesa A Canal	11.3	--	2.23	1.13	8.2	8.6
Trapezoidal Laboratory Channel with roughened sides	0.115	1.31	0.82	0.066	1.3	174
	0.154	1.41	1.48	0.118	2.7	150
	0.115	1.31	1.48	0.115	4.5	338
	0.115	1.12	1.44	0.114	0.8	205
	0.069	1.08	1.48	0.108	4.3	392
	0.069	0.62	1.51	0.127	2.4	270
Green-Duwamish River	3.61	66	--	0.16	70-92	120-160
Missouri River	8.86	660	5.09	0.24	16,000	7500
Copper Creek (below gage)	1.61	52	0.89	0.26	215	500
	2.79	59	1.97	0.33	226	250
	1.61	52	0.85	0.26	102	245
Clinch River	2.79	154	1.05	0.22	151	235
	6.89	197	3.08	0.34	581	245
	6.89	174	2.62	0.35	506	210
Copper Creek (above gage)	1.31	62	0.52	0.38	97	220
Powell River	2.79	112	0.49	0.18	102	200
Clinch River	1.90	118	0.69	0.16	87	280
Coachella Canal	5.12	79	2.33	0.14	103	140
Bayon Anacoco	3.08	85	1.12	0.22	355	524
	2.98	121	1.31	0.22	420	640
Nooksack River	2.49	210	2.20	0.89	377	170
Wind/Bighorn Rivers	3.61	194	2.89	0.39	452	318
	7.09	226	5.09	0.56	1722	436
John Day River	1.90	82	3.31	0.46	151	172
	8.10	112	2.69	0.59	700	146

TABLE II-2

EXPERIMENTAL MEASUREMENTS OF LONGITUDINAL DISPERSION IN OPEN CHANNELS

(After Table 5.3, Fischer et al. 1979) (Continued)

Channel	Depth d (ft)	Width W (ft)	Mean Velocity $\bar{u}$ (ft/sec)	Shear Velocity u^* (ft/sec)	Dispersion Coefficient D_l (ft^2/sec)	Dispersion Constant K
Comite River	1.41	52	1.21	0.16	151	650
Sabine River	6.69	341	1.90	0.16	3390	3100
	15.6	417	2.10	0.25	7200	1800
Yadkin River	7.71	230	1.41	0.33	1200	470
	12.6	236	2.49	0.43	2800	520

6

The model augments the stream flow by first comparing, after steady-state conditions have been reached, the simulated DO concentration with the prespecified target level of DO in each reach. If the calculated DO is below the target level, the program finds those upstream sources that the user has specified for dilution purposes, and adds water equally from all these sources. The DO calculations are then repeated. This process continues until the DO target level is satisfied. (NOTE: The flow augmentation subroutine can be used for DO only.)

3. CONSTITUENT REACTIONS AND INTERRELATIONSHIPS

3.1 GENERAL CONSIDERATIONS

One of the most important considerations in determining the waste-assimilative capacity of a stream is its ability to maintain an adequate dissolved oxygen concentration. Dissolved oxygen concentrations in streams are controlled by atmospheric reaeration, photosynthesis, plant and animal respiration, benthal demand, biochemical oxygen demand, nitrification, salinity, and temperature, among other factors.

The most accurate oxygen balance would consider all significant factors. The QUAL2E model includes the major interactions of the nutrient cycles, algae production, benthic oxygen demand, carbonaceous oxygen uptake, atmospheric aeration and their effect on the behavior of dissolved oxygen. Figure III-1 illustrates the conceptualization of these interactions. The arrows on the figure indicate the direction of normal system progression in a moderately polluted environment; the directions may be reversed in some circumstances for some constituents. For example, under conditions of oxygen supersaturation, which might occur as a result of algal photosynthesis, oxygen might be driven from solution, opposite to the indicated direction of the flow path.

Coliforms and the arbitrary nonconservative constituent are modeled as nonconservative decaying constituents and do not interact with other constituents. The conservative constituents, of course, neither decay nor interact in any way with other constituents.

The mathematical relationships that describe the individual reactions and interactions are presented in the following paragraphs.

3.2 CHLOROPHYLL $\underline{a}$ (PHYTOPLANKTONIC ALGAE)

Chlorophyll $\underline{a}$ is considered to be directly proportional to the concentration of phytoplanktonic algal biomass. For the purposes of this model, algal biomass is converted to chlorophyll $\underline{a}$ by the simple relationship

$$Chl\underline{a} = \alpha_0 A \qquad \text{III-1}$$

where

Chla = chlorophyll a concentration, ug-Chla/L

A = algal biomass concentration, mg-A/L

α_0 = a conversion factor, ug Chla/mg A

The differential equation that governs the growth and production of algae (chlorophyll a) is formulated according to the following relationship

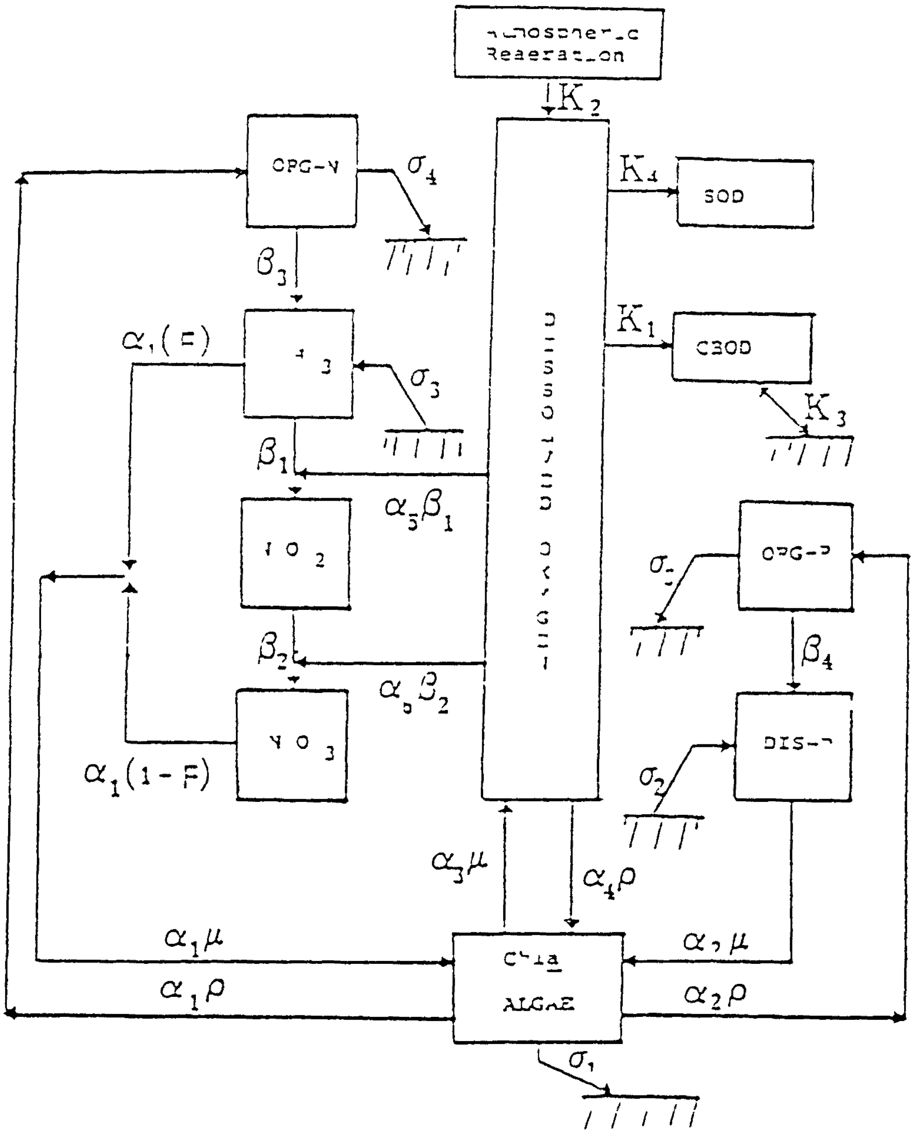


Figure III- Major Constituent interactions in QUAL2E

$$\frac{dA}{dt} = \mu A - \rho A - \frac{\sigma_1}{d} A \qquad \text{-2}$$

where

A = algal biomass concentration, mg-A/L

t = time, day

μ = the local specific growth rate of algae as defined below, which is temperature dependent, day^{-1}

ρ = the local respiration rate of algae, which is temperature dependent, day^{-1}

σ_1 = the local settling rate for algae, which is temperature dependent, ft/day

d = average depth, ft

3 2 1 Algal Respiration Rate

In QUAL2E, the single respiration rate parameter, ρ, is used to approximate three processes (a) the endogenous respiration of algae, (b) the conversion of algal phosphorus to organic phosphorus, and (c) the conversion of algal nitrogen to organic nitrogen No attempt is made to use separate rate coefficients for these three processes, as is done in the State of Vermont, revised Meta Systems version of QUAL-II (JRB Associates, 1983, and Walker, 1981)

3 2 2 Algal Specific Growth Rate

The local specific growth rate of algae, μ, is known to be coupled to the availability of required nutrients (nitrogen and phosphorus) and light A variety of mathematical expressions for expressing multiple nutrient-light limitations on algal growth rate have been reported (De Groot, 1983, Scavia and Park, 1976, and Swartzman and Bentley, 1979) QUAL2E has the capability of modeling the interaction among these limiting factors in three different ways

Growth Rate Option 1 Multiplicative The kinetic expressions used to represent the effects of nitrogen, phosphorus, and light are multiplied together to determine their net effect on the local algal growth rate This option has as its biological basis the multiplicative effects of enzymatic processes involved in photosynthesis

$$\mu = \mu_{max} \, (FL) \, (FN) \, (FP) \qquad \text{III-3a}$$

where

μ_{max} = maximum specific algal growth rate, day^{-1}

FL = algal growth limitation factor for light

FN = algal growth limitation factor for nitrogen

FP = algal growth limitation factor for phosphorus

This formulation is used in the SEMCOG version of QUAL-II

Growth Rate Option 2 Limiting Nutrient This option represents the local algal growth rate as limited by light and either nitrogen or phosphorus, but not both Thus, the nutrient/light effects are multiplicative, but the nutrient/nutrient effects are alternate This formulation mimics Liebig's law of the minimum

$$\mu = \mu_{max} (FL) \; \mathrm{Min} \; (FN, FP) \qquad \text{III-3b}$$

Thus, the algal growth rate is controlled by the nutrient (N or P) with the smaller growth limitation factor This option is used in the State of Vermont version of QUAL-II

Growth Rate Option 3 Harmonic Mean This option, a compromise between options 1 and 2, is a modification of an intuitive form suggested by Scavia and Park (1976) and is mathematically analogous to the total resistance of two resistors in parallel In this option, an effective nutrient limitation factor is computed as the average of the inverse reciprocals of the individual nitrogen and phosphorus growth limitation factors, i e ,

$$\mu = \mu_{max} (FL) \left[\frac{2}{1/FN + 1/FP} \right] \qquad \text{III-3c}$$

Thus, the algal growth rate is controlled by a multiplicative relation between light and nutrients, but the nutrient/nutrient interactions are represented by a harmonic mean This option has been used by Water Resources Engineers in the application of a QUAL-II-like model, WREDUN, to Lake Dunlap (Brandes and Stein, no date see also Bowie *et al* , 1985)

Walker (1983) has cautioned against using the harmonic mean option in systems where one nutrient is in excess (say nitrogen, so that $FN \rightarrow 1.0$) and the other is extremely limiting (say phosphorus, so that $FP \rightarrow 0.0$) In this case the value of the nutrient attenuation factor approaches 2 FP, rather than FP, as expected

3 2 3 Algal-Light Relationships

3 2 3 1 Light Functions

A variety of mathematical relationships between photosynthesis and light have been reported in the literature (Jassby and Platt, 1976, Field and Effler, 1982) Although they differ in mathematical form, the relationships exhibit similar characteristics All show an increasing rate of photosynthesis with increasing light intensity up to a maximum or saturation value At high light intensities, some of the expressions exhibit photoinhibition, whereas others show photosynthetic activity remaining at the maximum rate

QUAL2E recognizes three options for computing the algal growth limitation factor for light, FL in Equations III-3a,b,c Light attenuation effects on the algal growth rate may be simulated using a Monod half-saturation method, Smith's function (Smith, 1936), or Steele's equation (Steele, 1962)

Light Function Option 1 Half Saturation In this option, the algal growth limitation factor for light is defined by a Monod expression

$$FL_z = \frac{I_z}{K_L + I_z} \qquad \text{III-4a}$$

where

FL_z = algal growth attenuation factor for light at intensity I_z

I_z = light intensity at a given depth (z), Btu/ft^2-hr

K_L = half saturation coefficient for light, Btu/ft^2-hr

z = depth variable, ft

Light Function Option 2 Smith's Function In this option, the algal growth limitation factor for light is formulated to include second order effects of light intensity

$$FL_z = \frac{I_z}{(K_L{}^2 + I_z{}^2)^{1/2}} \qquad \text{III-4b}$$

where

K_L = light intensity corresponding to 71% of the maximum growth rate, Btu/ft^2-hr

with the other terms as defined in Equation III-4a

Light Function Option 3 Steel's Equation This option incorporates an exponential function to model the effect of photoinhibition on the algal growth rate

$$FL_z = \left(\frac{I_z}{K_L}\right) \exp\left(1 - \frac{I_z}{K_L}\right) \qquad \text{III-4c}$$

where

K_L = saturation light intensity at which the algal growth rate is a maximum, Btu/ft^2-hr

with the other terms as defined in Equation III-4a

Note The parameter K_L, which appears in all three light function equations is defined differently in each

All of the light functions in Equations III-4a,b,c express the value of FL for an optically thin layer In QUAL2E photosynthesis occurs throughout the depth of the water column Light intensity varies with depth according to Beer's law

$$I_z = I \exp(-\lambda z) \qquad \text{III-5}$$

where

I_z = light intensity at a given depth (z), Btu/ft^2-hr

I = surface light intensity, Btu/ft^2-hr

λ = light extinction coefficient, ft^{-1}

z = depth variable, ft

When Equation III-5 is substituted into Equations III-4a,b,c and integrated over the depth of flow the depth-averaged light attenuation factor is obtained The resulting expressions for the three options are

Option 1 Half Saturation

$$FL = (1/\lambda d) \ln \left[\frac{K_L + I}{K_L + Ie^{-\lambda d}}\right] \qquad \text{III-6a}$$

K_L = light intensity at which growth rate is 50% of the maximum growth rate

Option 2 Smith's Function

$$FL = (1/\lambda d)\ \ln\left[\frac{I/K_L + (1 + (I/K_L)^2)^{1/2}}{(I/K_L)e^{-\lambda d} + (1 + ([I/K_L]e^{-\lambda d})^2)^{1/2}}\right] \qquad \text{III-6b}$$

K_L = light intensity at which growth rate is 71% of the maximum growth rate

Option 3 Steel's Equation

$$FL = \frac{2.718}{\lambda d}\left[e^{-(e^{-\lambda d(I/K_L)})} - e^{-I/K_L}\right] \qquad \text{III-6c}$$

K_L = light intensity at which growth rate is equal to the maximum growth rate

where

FL = depth-averaged algal growth attenuation factor for light

K_L = light saturation coefficient, Btu/ft^2-hr

λ = light extinction coefficient, ft^{-1}

d = depth of flow, ft

I = surface light intensity, Btu/ft^2-hr

The relative merits of these light functions are discussed by various authors (Bannister, 1974, Platt *et al.*, 1981, Swartzmann and Bentley, 1979, and Field and Effler, 1982). The half saturation method is the form used in the SEMCOG version of QUAL-II. Evidence shows that the use of Smith's function is preferrable over the half saturation method if photoinhibition effects are unimportant (Jassby and Platt, 1976). The mathematical forms of Equations III-4a,b,c are compared graphically in Figure III-2. All three equations have a single parameter, K_L, however, it is defined differently in each equation. In Figure III-2 the values of K_L are selected so that each curve passes through a common point, namely FL = 0.5 at I = 5 intensity units (i.e., a half saturation rate equal to 5 light intensity units).

3.2.3.2 Light Averaging Options

Steady state algal simulations require computation of an average value of FL, the growth attenuation factor for light, over the diurnal cycle.

There are four options in QUAL2E for computing this average. The options arise from combinations of situations regarding two factors:

- The source of the solar radiation data used in the computation, i.e., whether it is supplied externally by the user or calculated internally in the temperature heat balance.
- The nature of the averaging process, i.e., whether hourly values of FL are averaged, or a single daylight average value of solar radiation is used to estimate the mean value of FL.

The four daily light averaging options are defined below. In each case, the half saturation light function is used as an example; in practice any of the three light functions may be employed.

Option 1. FL is computed from one daylight average solar radiation value calculated in the steady state temperature heat balance.

$$FL = AFACT * f * FL_1 \qquad \text{III-7a}$$

$$FL_1 = \frac{1}{\lambda d} \ln \left[\frac{K_L + I_{alg}}{K_L + I_{alg} e^{-\lambda d}} \right] \qquad \text{III-7b}$$

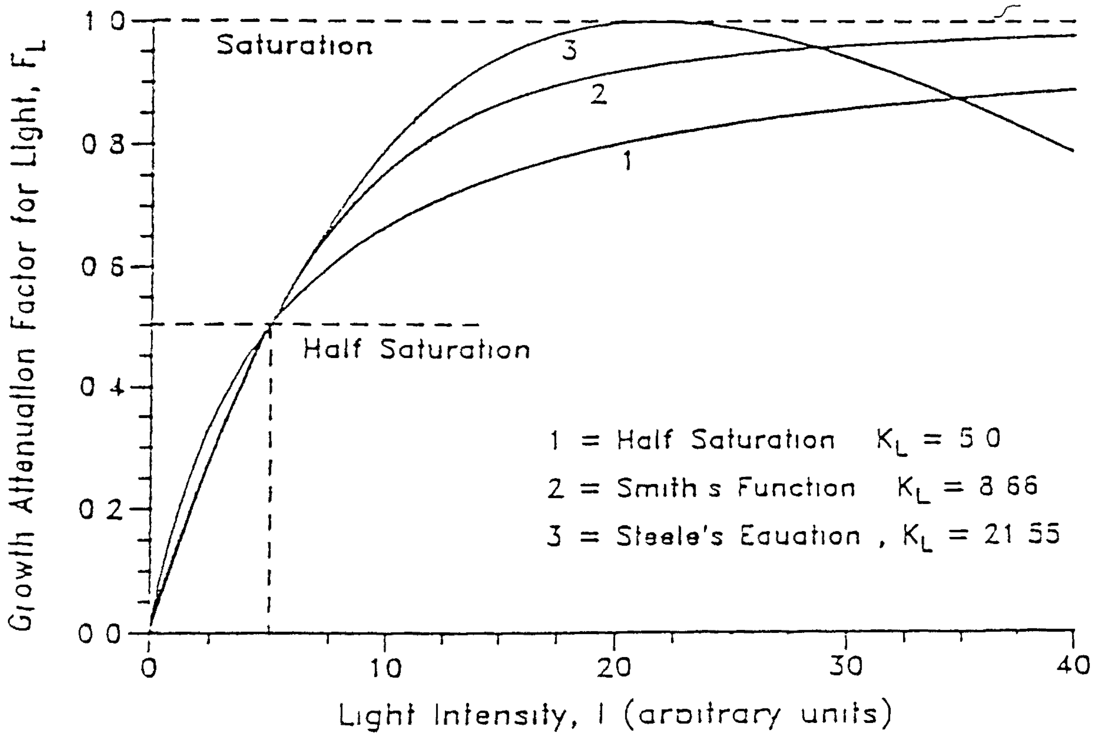


Figure III-2 QUAL2E Light Functions

$\overline{I}_{alg} = TFACT * \overline{I}_{temp}$ II-7c

where

FL = algae growth attenuation factor for light, adjusted for daylight hours and averaging method

AFACT = a light averaging factor, used to provide similarity between calculations using a single average value of solar radiation and computations using the average of hourly values of FL

f = fraction of daylight hours

FL_1 = growth attenuation factor for light, based on daylight average light intensity ($\overline{I}_{alg}$)

λ = light extinction coefficient, ft^{-1}

d = mean depth of stream, ft

K_L = half saturation coefficient for light, Btu/ft^2-hr

$\overline{I}_{alg}$ = daylight average, photosynthetically active, light intensity, Btu/ft^2-hr

TFACT = fraction of solar radiation computed in the temperature heat balance that is photosynthetically active

$\overline{I}_{temp}$ = daylight average light intensity as computed in the temperature heat balance, Btu/ft^2-hr

Option 2 FL is computed from one daylight average solar radiation value supplied externally by the user The calculations required to obtain FL in option 2 are the same as those for option 1, except that the value of $\overline{I}_{alg}$ is computed directly from user input of photosynthetically active sola radiation

$$\overline{I}_{alg} = I_{tot}/N \qquad \text{III-8}$$

where

I_{tot} = total daily photosynthetically active solar radiation, Btu/ft^2

N = number of daylight hours per day, hr

Both I_{tot} and N are supplied by the user as input information Equations III-8, III-7b, and III-7a are used to compute the value of FL Because the user input value of I_{tot} is assumed to be the photosynthetically active radiation, the factor TFACT is not used in option 2

Option 3 FL is obtained by averaging the hourly daylight values of FL that are computed from the hourly daylight values of solar radiation calculated in the steady state temperature heat balance

$$FL = f * FL_2 \qquad \text{III-9a}$$

$$FL_2 = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{\lambda d} \left[\frac{K_L + I_{alg,i}}{K_L + I_{alg,i} e^{-\lambda d}} \right] \qquad \text{III-9b}$$

$$I_{alg,i} = TFACT * I_{temp,i} \qquad \text{III-9c}$$

where

FL_2 = average of N hourly values of FL, based on hourly values of light intensity ($I_{alg,i}$)

$I_{alg,i}$ = hourly value of photosynthetically active light intensity, Btu/ft^2-hr

$I_{temp,i}$ = hourly value of light intensity as computed in the steady state temperature heat balance, Btu/ft^2-hr

with other terms are defined in Equations III-7a,b,c, and III-8

Because the average FL computed in option 3 (and 4) is an average of diurnally varying values of FL, the factor AFACT is not used in the calculations

Option 4 FL is obtained by averaging the hourly daylight values of FL that are computed from the hourly daylight values of solar radiation calculated from a single value of total daily, photosynthetically active, solar radiation and an assumed cosine function The calculations required to obtain FL are the same as those for option 3, except that the values of $I_{alg,i}$ are computed from an internally specified cosine function

$$I_{alg,i} = I_{tot}/N \left(1 - \cos \frac{2\pi i}{N + 1}\right), \quad i = 1,N \qquad \text{III-10}$$

As in the case of option 2, both I_{tot} and N are supplied by the user Equations III-10, III-9b, and III-9a are then used to compute the value of FL Because the user specified value of I_{tot} is assumed to be photosynthetically active, the factor TFACT is not used with option 4

Three empirical factors--diurnal cosine function, AFACT, and TFACT--are used in the formulations of the four light averaging options.

Two diurnal cosine functions were evaluated for use in QUAL2E: (1) a modified form of the one in the SEMCOG version of QUAL-II, and (2) the form used in QUAL-TX (Texas Water Development Board, 1984). The function in SEMCOG was modified to produce non-zero solar radiation values for each daylight hour, as given in Equation III-10. The form used in QUAL-TX is

$$I_{alg,i} = \frac{I_{tot}}{2N}\left[\cos\left(\frac{\pi(i-1)}{N}\right) - \cos\left(\frac{\pi i}{N}\right)\right], \qquad i=1,N \qquad \text{III-11}$$

Equations III-10 and III-11 were evaluated by comparing simulated values of FL from modeling options 2 and 4 (i.e., in effect computing values of AFACT). Simulations were performed over a range of values of K_L, λ, d, I_{tot}, and N, as well as for each of the three light functions. The values of AFACT averaged 0.92 and 0.94 for the SEMCOG and Texas equations, respectively. There was no compelling reason to include both functions (with the user specifying the one to be used). The diurnal cosine function used in QUAL2E, therefore, is the modified SEMCOG version given in Equation III-10.

AFACT is the adjustment factor accounting for the nonlinear averaging inherent in computing a daily average value of FL. From the simulations just described, a resonable value of AFACT is 0.92, with a range from 0.85 to 0.98. Bowie *et al.* (1985) report an implied value of 1.0 (Eq. 3.33), and Walker (1983) suggests using a value of 0.85.

TFACT is the photosynthetically active fraction of total solar radiation. When performing algae simulations, it is important that the value of light intensity and light saturation coefficient, K_L, be in units of photosynthetically active radiation, PAR (Bannister, 1974, Field and Effler, 1983, and Stefan *et al.*, 1983). Because the temperature heat balance computes total radiation over a wide spectrum, this value must be adjusted to PAR if it is to be used in the algae simulation. The ratio of energy in the visible band (PAR) to energy in the complete (standard) spectrum is approximately 0.43 to 0.45 (Bannister, 1974 and Stefan *et al.*, 1983). TFACT is a user input variable, thus a value to meet site specific conditions may be used.

Summary of Daily Averaging Options. The selection of a light averaging option depends largely on the extent to which the user wishes to account for the diurnal variation in light intensity. Options 1 and 2 use a single calculation of FL based on an "average" daily solar radiation value. Options 3 and 4 calculate hourly values of FL from hourly values of solar radiation and then average the hourly FL values to obtain the daily average value. Options 1 and 3 use the solar radiation from the temperature heat balance routines. (Thus both algae and temperature simulations draw on the same source for solar radiation.) Options 2 and 4 use the solar radiation value provided by the user for algae simulation. Thus, either option 2 or 4 must be selected when algae are simulated and temperature is not. The light averaging factor (AFACT) is used to provide similarity in FL calculations between options 1 and 2 versus options 3 and 4. The solar radiation factor (TFACT) specifies the fraction of the solar radiation computed in the heat balance, which is photosynthetically active. It is used only with options 1 or 3.

In dynamic algae simulations, photosynthetically active radiation is computed hourly using Equation III-9c unless temperature is not simulated, in which case photosynthetically active solar radiation data must be supplied with the local climatology data.

3.2.3.3 Algal Self Shading

The light extinction coefficient, λ, in Equations III-6a,b,c is coupled to the algal density using the nonlinear equation

$$\lambda = \lambda_0 + \lambda_1 \alpha_0 A + \lambda_2 (\alpha_0 A)^{2/3} \qquad \text{III-12}$$

where

λ_0 = non-algal portion of the light extinction coefficient, ft^{-1}

λ_1 = linear algal self shading coefficient, ft^{-1} $(ug\text{-}Chl\underline{a}/L)^{-1}$

λ_2 = nonlinear algal self shading coefficient, ft^{-1} $(ug\text{-}Chl\underline{a}/L)^{-2/3}$

α_0 = conversion factor, ug-Chl<u>a</u> /mg A

A = algal biomass concentration, mg-A/L

Appropriate selection of the values of λ_1 and λ_2 allows modeling of a variety of algal self-shading light-extinction relationships.

- No algal self shading (QUAL-II SEMCOG)

  $\lambda_1 = \lambda_2 = 0$

- Linear algal self shading (JRB Associates, 1983)

  $\lambda_1 \neq 0$, $\lambda_2 = 0$

- Nonlinear algal self shading (Riley Eq., in Bowie et al., 1985)

  $\lambda_1 = 0.00268$, ft^{-1} $(ug\text{-}Chl\underline{a}/L)^{-1}$

  $\lambda_2 = 0.0165$, ft^{-1} $(ug\text{-}Chl\underline{a}/L)^{-2/3}$

or

λ_1 = 0 0088, m^{-1} (ug-Chl$\underline{a}$/L$)^{-1}$

λ_2 = 0 054, m^{-1} (ug-Chl$\underline{a}$/L$)^{-2/3}$

3 2 4 Algal Nutrient Relationships

The algal growth limitation factors for nitrogen (FN) and for phosphorus (FP) are defined by the Monod expressions

$$FN = \frac{N_e}{N_e + K_N} \qquad \text{III-13}$$

and

$$FP = \frac{P_2}{P_2 + K_P} \qquad \text{III-14}$$

where

N_e = the effective local concentration of available inorganic nitrogen, mg-N/L

K_N = the Michaelis-Menton half-saturation constant for nitrogen, mg-N/L

P_2 = the local concentration of dissolved phosphorus, mg-P/L

K_P = the Michaelis-Menton half-saturation constant for phosphorus, mg-P/L

Algae are assumed to use ammonia and/or nitrate as a source of inorganic nitrogen The effective concentration of available nitrogen is given by

$$N_e = N_1 + N_3 \qquad \text{III-15}$$

where

N_1 = concentration of ammonia nitrogen, mg-N/L

N_3 = concentration of nitrate nitrogen, mg-N/L

The empirical half-saturation constants for nitrogen, K_N, and phosphorus, K_P, are used to adjust the algal growth rate to account for those factors that can potentially limit algal growth. Each constant is actually the level at which that particular factor limits algal growth to half the maximal or 'saturated' rate (Bowie et al., 1985). Table III-3 at the end of this chapter lists typical values of the half-saturation constants for nitrogen and phosphorus. If algal concentrations are simulated and either nitrogen, phorphorus or both are not simulated, the program assumes that the parameter not simulated is not limiting.

3.2.5 Temperature Dependence in Algae Simulation

The algal growth rate and death rates are temperature dependent. They are corrected within the model, as are all other temperature dependent systems variables, according to the procedure explained in Section 3.10.

3.3 NITROGEN CYCLE

In natural aerobic waters, there is a stepwise transformation from organic nitrogen to ammonia, to nitrite, and finally to nitrate. The nitrogen cycle in QUAL2E contains all four of these components, as shown in Figure III-1. The incorporation of organic nitrogen as a state variable, an organic nitrogen settling term, and an algal nitrogen uptake preference factor are the primary enhancements to the nitrogen cycle in QUAL2E compared to the SEMCOG version of QUAL-II. The differential equations governing transformations of nitrogen from one form to another are shown below.

3.3.1 Organic Nitrogen

$$\frac{dN_4}{dt} = \alpha_1 \rho A - \beta_3 N_4 - \sigma_4 N_4 \qquad \text{III-16}$$

where

N_4 = concentration of organic nitrogen, mg-N/L

β_3 = rate constant for hydrolysis of organic nitrogen to ammonia nitrogen, temperature dependent, day^{-1}

α_1 = fraction of algal biomass that is nitrogen, mg-N/mg-A

ρ = Algal respiration rate, day^{-1}

A = algal biomass concentration, mg-A/L

σ_4 = rate coefficient for organic nitrogen settling, temperature dependent, day^{-1}

3 3 2 Ammonia Nitrogen

$$\frac{dN_1}{dt} = \beta_3 N_4 - \beta_1 N_1 + \sigma_3/d - F_1 \alpha_1 \mu A \qquad \text{III-17}$$

where

$$F_1 = P_N N_1/(P_N N_1 + (1 - P_N) N_3) \qquad \text{III-18}$$

N_1 = the concentration of ammonia nitrogen, mg-N/L

N_3 = the concentration of nitrate nitrogen, mg-N/L

N_4 = the concentration of organic nitrogen, mg-N/L

β_1 = rate constant for the biological oxidation of ammonia nitrogen, temperature dependent, day^{-1}

β_3 = organic nitrogen hydrolysis rate, day^{-1}

α_1 = fraction of algal biomass which is nitrogen, mg-N/mg-A

σ_3 = the benthos source rate for ammonia nitrogen, mg-N/ft^2-day

d = mean depth of flow, ft

F_1 = fraction of algal nitrogen uptake from ammonia pool

μ = the local specific growth rate of algae, day^{-1}

A = algal biomass concentration, mg-A/L

P_N = preference factor for ammonia nitrogen (0 to 1.0)

The QUAL2E model includes an algal preference factor for ammonia, P_N (Bowie *et al.*, 1985, JRB Associates, 1983). The ammonia preference factor is equivalent to the fraction of algal nitrogen uptake from the ammonia pool when the concentrations of ammonia and nitrate nitrogen are equal.

3 3 3 Nitrite Nitrogen

$$\frac{dN_2}{dt} = \beta_1 N_1 - \beta_2 N_2 \qquad \text{III-19}$$

where

N_1 = the concentration of ammonia nitrogen, mg-N/L

N_2 = the concentration of nitrite nitrogen, mg-N/L

β_1 = rate constant for the oxidation of ammonia nitrogen, temperature dependent, day^{-1}

β_2 = rate constant for the oxidation of nitrite nitrogen, temperature dependent, day^{-1}

3 3 4 Nitrate Nitrogen

$$\frac{dN_3}{dt} = \beta_2 N_2 - (1 - F)\alpha_1 \mu A \qquad \text{III-20}$$

where

F = fraction of algal nitrogen taken from ammonia pool, as defined in Section 3 3 2

α_1 = fraction of algal biomass that is nitrogen, mg-N/mg-A

μ = local specific growth rate of algae, day^{-1}

3 3 5 Inhibition of Nitrification at Low Dissolved Oxygen

QUAL2E has the capability of inhibiting (retarding) the rate of nitrification at low values of dissolved oxygen This inhibition effect has been reported by others (Department of Scientific and Industrial Research, 1964, Texas Water Development Board, 1984)

Nitrification rates are modified in QUAL2E by computing an inhibition correction factor (having a value between zero and one) and then applying this factor to the values of the nitrification rate coefficients, β_1, and β_2 The nitrification rate correction factor is computed according to a first order equation

$$\text{CORDO} = 1.0 - \exp(-\text{KNITRF} * \text{DO}) \qquad \text{III-21}$$

where

CORDO = nitrification rate correction factor

exp = exponential function

KNITRF = first order nitrification inhibition coefficient, mg/L^{-1}

DO = dissolved oxygen concentration, mg/L

The correction factor is applied to the ammonia and nitrite oxidation rates by

Ammonia $(\beta_1)_{inhib}$ = CORDO * $(\beta_1)_{input}$ III-22

Nitrite $(\beta_2)_{inhib}$ = CORDO * $(\beta_2)_{input}$ III-23

A value of 0.6 for KNITRF closely matches the inhibition formulation in QUAL-TX, the Texas Water Development Board version of QUAL-II, whereas, a value of 0.7 closely simulates the data for the Thames Estuary (DSIR, 1964).

3.4 PHOSPHORUS CYCLE

The phosphorus cycle operates like the nitrogen cycle in many respects. Organic forms of phosphorus are generated by the death of algae, which then convert to the dissolved inorganic state, where it is available to algae for primary production. Phosphorus discharged from sewage treatment plants is generally in the dissolved inorganic form and is readily taken up by algae (Bowie *et al.*, 1985). QUAL2E revises the SEMCOG version of QUAL-II, which included only dissolved phosphorus, to simulate the interactions between organic and dissolved phosphorus. Below are the differential equations governing transformations of phosphorus from one form to another.

3.4.1 Organic Phosphorus

$$\frac{dP_1}{dt} = \alpha_2 \rho A - \beta_4 P_1 - \sigma_5 P_1 \qquad \text{III-24}$$

where

P_1 = the concentration of organic phosphorus, mg-P/L

α_2 = phosphorus content of algae, mg P/mg-A

ρ = algal respiration rate, day^{-1}

A = algal biomass concentration, mg-A/L

β_4 = organic phosphorus decay rate, temperature dependent, day^{-1}

σ_5 = organic phosphorus settling rate, temperature dependent, day^{-1}

3 4 2 Dissolved Phosphorus

$$\frac{dP_2}{dt} = \beta_4 P_1 + \sigma_2/d - \alpha_2 \mu A \qquad \text{I-25}$$

where

P_2 = concentration of inorganic or dissolved phosphorus, mg-P/L

σ_2 = benthos source rate for dissolved phosphorus, temperature dependent, mg-P/ft^2-day

d = mean stream depth, ft

μ = algal growth rate, day^{-1}

A = algal biomass concentration, mg-A/L

3 5 CARBONACEOUS BOD

The QUAL2E model assumes a first order reaction to describe deoxygenation of ultimate carbonaceous BOD in the stream The BOD function as expressed in the model also takes into account additional BOD removal due to sedimentation, scour and flocculation, which do not exert an oxygen demand (Thomas, 1948)

$$\frac{dL}{dt} = - K_1 L - K_3 L \qquad \text{III-26}$$

where

L = the concentration of ultimate carbonaceous BOD, mg/L

K_1 = deoxygenation rate coefficient, temperature dependent, day^{-1}

K_3 = the rate of loss of carbonaceous BOD due to settling, temperature dependent, day^{-1}

QUAL2E simulates ultimate BOD in the general case, however, the user may choose to use 5-day BOD values for input and output In this case, the model will make the necessary coversions from 5-day to ultimate BOD The conversion equation is

$$BOD_5 = BOD_u\ (1\ 0 - \exp(5 * KBOD)) \qquad \text{III-27}$$

where

BOD_5 = 5-day BOD, mg/L

BOD_u = ultimate BOD, mg/L

KBOD = BOD conversion rate coefficient, day^{-1}

The SEMCOG version of QUAL-II uses a value of 0 23 day^{-1} for KBOD Wi QUAL2E, the user may specify the appropriate value for this conversion No when modeling 5-day BOD, the same conversion coefficient is applied to all input BOD_5 forcing functions (headwaters, incremental flows, point loads, a the downstream boundary condition)

3 6 DISSOLVED OXYGEN

The oxygen balance in a stream system depends on the capacity of the stream to reaerate itself This capacity is a function of the advection and diffusion processes occurring within the system and the internal sources and sinks of oxygen The major sources of oxygen, in addition to atmospheric reaeration, are the oxygen produced by photosynthesis and the oxygen contai in the incoming flow The sinks of dissolved oxygen include biochemical oxidation of carbonaceous and nitrogenous organic matter, benthic oxygen demand and the oxygen utilized by algae respiration (Bowie <u>et al</u> , 1985)

The differential equation used in QUAL2E to describe the rate of change of oxygen is shown below Each term represents a major source or sink of oxygen

$$\frac{dO}{dt} = K_2(O^*-O) + (\alpha_3 \mu - \alpha_4 \rho) A - K_1 L - K_4/d - \alpha_5 \beta_1 N_1 - \alpha_6 \beta_2 N_2 \qquad \text{III-28}$$

where

O = the concentration of dissolved oxygen, mg/L

O* = the saturation concentration of dissolved oxygen at the local temperature and pressure, mg/L

α_3 = the rate of oxygen production per unit of algal photosynthesis, mg-O/mg-A

α_4 = the rate of oxygen uptake per unit of algae respired, mg-O/mg-A

α_5 = the rate of oxygen uptake per unit of ammonia nitrogen oxidation, mg-O/mg-N

α_6 = the rate of oxygen uptake per unit of nitrite nitrogen oxidation, mg-O/mg-N

μ = algal growth rate, temperature dependent, day^{-1}

ρ = algal respiration rate, temperature dependent, day^{-1}

A = algal biomass concentration, mg-A/L

L = concentration of ultimate carbonaceous BOD, mg/L

d = mean stream depth, ft

K_1 = carbonaceous BOD deoxygenation rate, temperature dependent, day^{-1}

K_2 = the reaeration rate in accordance with the Fickian diffusion analogy, temperature dependent, day^{-1}

K_4 = sediment oxygen demand rate, temperature dependent, g/ft^2-day

β_1 = ammonia oxidation rate coefficient, temperature dependent, day^{-1}

β_2 = nitrite oxidation rate coefficient, temperature dependent, day^{-1}

N_1 = ammonia nitrogen concentration, mg-N/L

N_2 = nitrite nitrogen concentration, mg-N/L

3.6.1 Dissolved Oxygen Saturation Concentration

The solubility of dissolved oxygen in water decreases with increasing temperature, increasing dissolved solids concentration, and decreasing atmospheric pressure (Bowie et al., 1985). QUAL2E uses a predictive equation for the saturation (equilibrium) concentration of dissolved oxygen (APHA, 1985).

$$\ln O^* = -139.34410 - (1.575701 \times 10^5/T) - (6.642308 \times 10^7/T^2) + (1.243800 \times 10^{10}/T^3) - (8.621949 \times 10^{11}/T^4) \qquad \text{III-29}$$

where

O^* = equilibrium oxygen concentration at 1.000 atm, mg/L

T = temperature (°K) = (°C-273.150) and °C is within the range 0.0 to 40.0°C

For non-standard conditions of pressure, the equilibrium concentration of dissolved oxygen is corrected by the equation III-30

$$Op = O^{*}P \left[\frac{(1 - P_{wv}/P)\,(1 - \theta P)}{(1 - P_{wv})\,(1 - \theta)} \right] \qquad \text{III-30}$$

where

Op = equilibrium oxygen concentration at non-standard pressure, mg/L

O* = equilibrium oxygen concentration at 1.000 atm, mg/L

P = pressure (atm) and is within 0.000 to 2.000 atm

P_{wv} = partial pressure of water vapor (atm), which may be computed from

$$\ln P_{wv} = 11.8571 - (3840.70/T) - 216961/T^2) \qquad \text{III-31}$$

and

$$\theta = 0.000975 - (1.426 \times 10^{-5} t) - (6.436 \times 10^{-8} t^2) \qquad \text{II-32}$$

where

t = temperature, °C

The equations in Standard Methods (1985) for computing dissolved oxygen saturation concentrations also include corrections for salinity and chloride. Because neither salinity nor chloride is explicitly modeled, QUAL2E does not correct O* for chloride or salinity. Furthermore, the pressure correction to O* (Equation III-30) is made only when temperature is modeled, because barometric pressure data are a primary requirement of the heat balance equations.

The dissolved oxygen saturation concentrations computed from the Texas and SEMCOG versions of QUAL-II are compared to those from the Standard Methods formulations of QUAL2E in Table III-1.

3.6.2 Atmospheric Reaeration Coefficient Estimation

The reaeration coefficient (K_2) is most often expressed as a function of stream depth and velocity. QUAL2E provides eight options for estimating or reading in K_2 values, which are discussed in the sections below. A comparative study of reaeration prediction equation performance has been reported by St. John et al. (1984).

TABLE III-1
COMPARISON OF DISSOLVED OXYGEN SATURATION CONCENTRATIONS
(Barometric Pressure = 1 atm, Chloride = 0 0mg/L, Equilibrium with Air Saturated with Water Vapor)

Temperature, °C	QUAL- I SEMCOG	QUAL-TX Texas	QUAL2E Std Meth
0	14.631	14.584	14.621
1	14.227	14.187	14.217
2	13.837	13.806	13.830
3	13.461	13.441	13.461
4	13.100	13.091	13.108
5	12.752	12.755	12.771
6	12.418	12.433	12.448
7	12.096	12.124	12.139
8	11.787	11.828	11.843
9	11.489	11.544	11.560
10	11.203	11.271	11.288
11	10.927	11.009	11.027
12	10.661	10.758	10.777
13	10.406	10.517	10.537
14	10.159	10.285	10.306
15	9.922	10.062	10.084
16	9.692	9.848	9.870
17	9.471	9.642	9.665
18	9.257	9.444	9.467
19	9.050	9.253	9.276
20	8.849	9.069	9.093
21	8.655	8.891	8.915
22	8.465	8.720	8.744
23	8.281	8.555	8.578
24	8.101	8.396	8.418
25	7.925	8.241	8.264
26	7.753	8.092	8.114
27	7.584	7.948	7.969
28	7.417	7.807	7.828
29	7.252	7.672	7.691
30	7.089	7.540	7.559
31	6.927	7.412	7.430
32	6.765	7.288	7.305
33	6.604	7.167	7.183
34	6.442	7.049	7.065
35	6.280	6.935	6.949
36	6.116	6.823	6.837
37	5.950	6.715	6.727
38	5.782	6.609	6.620
39	5.612	6.506	6.515
40	5.438	6.406	6.413

K_2 Option 1

Option 1 allows the user to read in K_2 values that have been previou selected by the modeler. This option is useful in modeling unusual situa such as ice cover (see Section 3.6.3).

K_2 Option 2

Using data collected in field measurements of stream reaeration, Churchill, Elmore, and Buckingham (1962) developed the following expressio for K_2 at 20°C

$$K_2^{20} = 5.026 \, \bar{u}^{0.969} \, d^{-1.673} \times 2.31 \qquad \text{III-33}$$

where

$\bar{u}$ = average velocity in the stream, ft/sec

d = average depth of the stream, ft

K_2 = reaeration coefficient, day^{-1}

K_2 Option 3

O'Connor and Dobbins (1958) proposed equations based on the turbulence characteristics of a stream. For streams displaying low velocities and isotropic conditions, Equation III-34 was developed

$$K_2^{20} = \frac{(D_m \, \bar{u})^{0.5}}{d^{1.50}} \qquad \text{III-34}$$

For streams with high velocities and nonisotropic conditions, the relationship is

$$K_2^{20} = \frac{480 D_m^{0.5} \, S_o^{0.25}}{d^{1.25}} \times 2.31 \qquad \text{III-35}$$

where

S_o = slope of the streambed, ft/ft

d = mean stream depth, ft

$\bar{u}$ = mean velocity, ft/day

K_2 = reaeration coefficient, day^{-1}

and D_m is the molecular diffusion coefficient (ft^2/day), which is given by

$$D_m = 1.91 \times 10^3 \; (1.037)^{T-20} \qquad \text{III-36}$$

Equation III-34 has been found to be generally applicable for most cases and is the equation used in QUAL2E for Option 3. Equation III-35 can be used to calculate K_2 outside the model and input it directly under Option 1.

K_2 Option 4

Based on the monitoring of six streams in England, Owens et al. (1964) obtained reaeration estimates for shallow, fast moving streams. Combining their data with that of Churchill et al., they developed an equation for streams exhibiting depths of 0.4 to 11.0 feet and velocities of 0.1 to 5.0 ft/sec

$$K_2^{20} = 9.4 \; \bar{u}^{0.67} / d^{1.85} \times 2.31 \qquad \text{III-37}$$

where

$\bar{u}$ = mean velocity, ft/sec

d = mean depth, ft

K_2 Option 5

Thackston and Krenkel (1966) proposed the following equation based on their investigation of several rivers in the Tennessee Valley Authority system

$$K_2^{20} = 10.8 \; (1 + F^{0.5}) \; \frac{u^*}{d} \times 2.31 \qquad \text{III-38}$$

where F is the Froude number, which is given by

$$F = \frac{u^*}{\sqrt{g\,d}} \qquad \text{III-39}$$

and u^* is the shear velocity, ft/sec

$$u^* = \sqrt{d \, S_e g} = \frac{\bar{u} \, n \sqrt{g}}{1.49 \, d^{1.167}} \qquad \text{III-40}$$

where

d = mean depth, ft

g = acceleration of gravity, ft/sec^2

S_e = slope of the energy gradient

$\overline{u}$ = mean velocity, ft/sec

n = Manning's coefficient

K_2 Option 6

Langbien and Durum (1967) developed a formula for K_2 at 20°C

$$K_2^{20} = 3.3\ \overline{u}/d^{1.33} \times 2.31 \qquad \text{III-41}$$

where

$\overline{u}$ = mean velocity, ft/sec

d = mean depth, ft

K_2 Option 7

This option computes the reaeration coefficient from a power function of flow. This empirical relationship is similar to the velocity and depth correlations with flow used in the hydraulics section of QUAL2E, i.e.,

$$K_2 = aQ^b \qquad \text{III-42}$$

where

a = coefficient of flow for K_2

Q = flow, ft^3/sec

b = exponent on flow for K_2

K_2 Option 8

The method of Tsivoglou and Wallace (1972) assumes that the reaeration coefficient for a reach is proportional to the change in elevation of the water surface in the reach and inversely proportional to the flow time through the reach. The equation is

$$K_2^{20} = c \frac{\Delta h}{t_f} \qquad \text{III-43}$$

where

c = escape coefficient, ft^{-1}

Δh = change in water surface elevation in reach, ft

t_f = flow time within reach, days

Assuming uniform flow, the change in water surface elevation is

$$\Delta h = S_e \, \Delta x \qquad \text{III-44}$$

where

S_e = slope of the energy gradient, ft/ft

Δx = reach length, ft

and the time of passage through a reach is

$$t_f = \frac{\Delta x}{\overline{u}} \qquad \text{III-45}$$

where

$\overline{u}$ = mean velocity in reach, ft/sec

Substituting the above in equation III-43 gives

$$K_2^{20} = (3600 \times 24) \, c S_e \, \overline{u} \qquad \text{III-46}$$

Equation III-46 is the form of Option 8 used in QUAL2E. The constants 3600 and 24 convert velocity to units of feet per day. The slope may be input directly for computing K_2 with this option, or it can be calculated from Manning's equation as follows

$$S_e = \frac{\overline{u}^2 \, n^2}{(1.49)^2 \, d^{4/3}} \qquad \text{III-47}$$

where

d = mean depth, ft

n = Manning's coefficient

The escape coefficient is usually treated as a variable and determined empirically TenEch (1978) recommends the following guideline in determining c values, analogous to that recommended for uncalibrated stream segments by Tsivoglou and Neal (1976)

$c = 0\ 054\ ft^{-1}$ (at 20°C) for $15 <= Q <= 3000\ ft^3/sec$

$c = 0\ 110\ ft^{-1}$ (at 20°C) for $1 <= Q <= 15\ ft^3/sec$

3 6 3 Ice Cover

Ice cover on streams during winter low flow conditions may significantly affect reaeration Reaeration rates are decreased because ice cover reduces the surface area of the air-water interface through which reaeration occurs (TenEch, 1978) Approaches recommended by TenEch (1978) for estimating the extent of ice cover include

- Statistical analyses of past records
- Steady state heat budget analysis (including the U S Army Corps of Engineers differential equations)
- Extensive field observations

To adjust the reaeration rate for winter ice cover conditions in the QUAL2E model, the calculated reaeration rate must be multiplied by an "ice cover factor" and input under Option 1 TenEch recommends factors ranging from 0 05 for complete ice cover to 1 0 for no ice cover Depending on the extent of cover, reaeration values can be greatly reduced

3 6 4 K_2 Default Values

There are no default K_2 values in QUAL2E In some versions of QUAL-II, a default value of K_2 is computed, accounting for the influences of wind-induced turbulence and difusion under low-velocity conditions In those models, when the calculated values of K_2 are less than two divided by the depth of the reach (2/d), K_2 is set equal to 2/d This feature has not always proved useful, particularly when simulating the very low reaeration rates, thus it is not included in QUAL2E

3.6.5 Dam Reaeration

QUAL2E has the capability of modeling oxygen input to the system from reaeration over dams. The following equation described by Butts and Evans (1983) and attributable to Gameson is used to estimate oxygen input from dam reaeration

$$D_a - D_b = [1 - \frac{1}{1 + 0.116abH(1 - 0.034H)(1 + .046T)}] D_a \qquad \text{III-48}$$

where

D_a = oxygen deficit above dam, mg/L

D_b = oxygen deficit below dam, mg/L

T = temperature, °C

H = height through which water falls, ft

a = empirical water quality factor

= 1.80 in clean water

= 1.60 in slightly polluted water

= 1.0 in moderately polluted water

= 0.65 in grossly polluted water

b = empirical dam aeration coefficients

= 0.70 to 0.90 for flat broad crested weir

= 1.05 for sharp crested weir with straight slope face

= 0.80 for sharp crested weir with vertical face

= 0.05 for sluice gates with submerged discharge

The factors H, a and b are input for each dam. The model includes a provision for bypassing some or all of the flow around the dams (e.g., through generators). The fraction of the total flow that spills over the dam is supplied as an input variable.

3.7 COLIFORMS

Coliforms are used as an indicator of pathogen contamination in surface waters. Expressions for estimating coliform concentrations are usually first order decay functions, which only take into account coliform die-off (Bowie *et al.*, 1985). The QUAL2E model uses such an expression

$$\frac{dE}{dt} = -k_5 E \qquad \text{III-49}$$

where

E = concentration of coliforms, colonies/100 ml

k_5 = coliform die-off rate, temperature dependent, day^{-1}

3.8 ARBITRARY NONCONSERVATIVE CONSTITUENT

QUAL2E has the provision for modeling an arbitrary nonconservative constituent (ANC). In addition to a first order decay mechanism, there are source and sink terms in the mass balance. The differential equation describing the interactions for an arbitrary nonconservative constituent is

$$\frac{dP}{dt} = -k_6 P - \sigma_6 P + \sigma_7/d \qquad \text{III-50}$$

where

P = concentration of the nonconservative constituent, mg-ANC/L

k_6 = decay rate for the constituent, temperature dependent, day^{-1}

σ_6 = rate coefficient for constituent settling, temperature dependent, day^{-1}

σ_7 = benthal source for constituent, temperature dependent, mg-ANC/ft^2-day

d = mean stream depth, ft

3.9 TEMPERATURE

Temperature is modeled by performing a heat balance on each computational element in the system. The heat balance accounts for temperature inputs and losses from the forcing functions as well as the heat exchanged between the water surface and the atmosphere. The air-water heat balance terms include long and short wave radiation, convection, and evaporation using

$$H_n = H_{sn} - H_{an} - H_b - H_c - H_e \qquad \text{III-51}$$

where

H_n = net heat flux passing the air water surface, Btu/ft^2-day

H_{sn} = net short wave solar radiation after losses from absorption and scattering in the atmosphere and by reflection at the interface, Btu/ft^2-day

H_{an} = net long wave atmosphere radiation after reflection, Btu/ft^2-day

H_b = outgoing long wave back radiation, Btu/ft^2-day

H_c = convective heat flux, Btu/ft^2-day

H_e = heat loss by evaporation, excluding sensible heat loss, Btu/ft^2-day

In order for QUAL2E to perform the heat balance computations, the user must supply a variety of data, including the longitude and latitude of the basin, the time of year, evaporation coefficients, and a dust attenuation coefficient Local climatological information in the form of time of day, wet and dry bulb air temperatures, atmospheric pressure, cloud cover and wind velocity also must be provided

In the dynamic mode, local climatological data must be supplied at regular (typically 3 hour) intervals In this manner the source/sink term for the heat balance is updated in time to simulate the diurnal response of the steady hydraulic system to changing temperature conditions

In the steady state mode, average local climatological data must be supplied by the user The program uses linear approximations for the long-wave back radiation and evaporation terms for solution of the steady state heat balance The reader is referred to Chapter 1 of this report for a detailed treatment of the temperature simulation

In the dynamic mode, local climatology data are applied uniformly over the entire river basin (i e , there is no spatial variation) In the steady state mode, local climatology data may vary spatially by reach

3 10 TEMPERATURE DEPENDENCE OF RATE COEFFICIENTS

The temperature values computed in QUAL2E are used to correct the rate coefficients in the source/sink terms for the other water quality variables These coefficients are input at 20°C and are then corrected to temperature using a Streeter-Phelps type formulation

$$X_T = X_{20}\,\theta^{(T-20°)} \qquad \text{III-52}$$

where

X_T = the value of the coefficient at the local temperature (T)

X_{20} = the value of the coefficient at the standard temperature (20°C)

θ = an empirical constant for each reaction coefficient

The values of the temperature correction factors, θ, may be specified by the user. In the absence of user specified values, the default values shown in Table III-2 are employed. For comparison purposes, the θ values used in the SIMCOS version of QUAL-II are also listed in Table III-2.

If temperature is not simulated, the temperature value specified for the initial condition is assumed to be the temperature for the simulation.

3.11 REACTION RATES AND PHYSICAL CONSTANTS

The chemical and biological reations that are simulated by QUAL2E are represented by a complex set of equations that contain many system parameter some are constant, some are spatially variable, and some are temperature dependent. Table III-3 lists these system parameters and gives the usual range of values, units, and types of variation. Kramer (1970), Chen and Orlob (1972), and Bowie et al. (1985) give detailed discussions of the basic sources of data, ranges and reliabilities of each of these parameters. Fina selection of the values for many of these system parameters or measurement o sensitive ones should be made during model calibration and verification.

TABLE III-2
DEFAULT TEMPERATURE CORRECTION, θ VALUES FOR QUAL2E

Rate Coefficient	Symbol	Default Values	
		SEMCOG	QUAL2E
BOD Decay	K_1	1 047	1 047
BOD Settling	K_3	-	1 024
Reaeration	K_2	1 0159	1 024
SOD Uptake	K_4	-	1 060
Organic N Decay	β_3	-	1 047
Organic N Settling	σ_4	-	1 024
Ammonia Decay	β_1	1 047	1 083
Ammonia Source	σ_3	-	1 074
Nitrite Decay	β_2	1 047	1 047
Organic P Decay	β_4	-	1 047
Organic P Settling	σ_5	-	1 024
Dissolved P Source	σ_2	-	1 074
Algal Growth	μ	1 047	1 047
Algal Respiration	ρ	1 047	1 047
Algal Settling	σ_1	-	1 024
Coliform Decay	K_5	1 047	1 047
ANC	K_6	1 047	1 000
ANC	σ_5	-	1 024
ANC	σ_7	-	1 000

Note - = not temperature dependent in QUAL-II SEMCOG

ANC = Arbitrary Nonconservative Constituent

TABLE [illegible]
TYPICAL RANGES FOR QUAL2E REACTION COEFFICIENTS

Variable	Description	Units	Range of Values	Variable by Reach	Temperatu Dependen
α_0	Ratio of chlorophyll-a to algal biomass	$\frac{\mu g\text{-}Chla}{mg\ A}$	10-100	No	No
α_1	Fraction of algal biomass that is Nitrogen	$\frac{mg\text{-}N}{mg\ A}$	0.07-0.09	No	No
α_2	Fraction of algal biomass that is Phosphorus	$\frac{mg\text{-}P}{mg\ A}$	0.01-0.02	No	No
α_3	O_2 production per unit of algal growth	$\frac{mg\text{-}O}{mg\ A}$	1.4-1.8	No	No
α_4	O_2 uptake per unit of algae respired	$\frac{mg\text{-}O}{mg\ A}$	1.6-2.3	No	No
α_5	O_2 uptake per unit of NH_3 oxidation	$\frac{mg\text{-}O}{mg\ N}$	3.0-4.0	No	No
α_6	O_2 uptake per unit of NO_2 oxidation	$\frac{mg\text{-}O}{mg\ N}$	1.0-1.14	No	No
μ_{max}	Maximum algal growth rate	day^{-1}	1.0-3.0	No	No
ρ	Algal respiration rate	day^{-1}	0.05-0.5	No	No
K_L	Michaelis-Menton half-saturation constant for light (Option 1)	$Btu/ft^2\text{-}min$	0.02-0.10	No	No
K_N	Michaelis-Mention half-saturation constant for nitrogen	mg-N/L	0.01-0.30	No	No
K_P	Michaelis-Menton half-saturation constant for phosphorus	mg-P/L	0.01-0.05	No	No
λ_0	Non-algal light extinction coefficient	ft^{-1}	Variable	No	No
λ_1	Linear algal self-shading coefficient	$\frac{1/ft}{\mu g\ Chla/L}$	0.002-0.02	No	No

TABLE III-3 (cont'd)
TYPICAL RANGES FOR QUAL2E REACTION COEFFICIENTS

Variable	Description	Units	Range of Values	Variable by Reach	Temperature Dependent
λ_2	Nonlinear algal self-shading coefficient	$\frac{1/ft}{(\mu g\ Chl\underline{a}/L)^{2/3}}$	0.0165 (Riley)	No	No
P_N	Algal preference factor for ammonia	-	0.0-1.0	No	No
σ_1	Algal settling rate	ft/day	0.5-6.0	Yes	Yes
σ_2	Benthos source rate for dissolved phosphorus	$\frac{mg\text{-}P}{ft^2\text{-}day}$	Variable	Yes	Yes
σ_3	Benthos source rate for ammonia nitrogen	$\frac{mg\text{-}O}{ft^2\text{-}day}$	Variable	Yes	Yes
σ_4	Organic nitrogen settling rate	day^{-1}	0.001-0.1	Yes	Yes
σ_5	Organic phosphorus settling rate	day^{-}	0.001-0.1	Yes	Yes
σ_6	Arbitrary non-conservative settling rate	day^{-1}	Variable	Yes	Yes
σ_7	Benthal source rate for arbitrary non-conservative settling rate	$\frac{mg\text{-}ANC}{ft^2\text{-}day}$	Variable	Yes	Yes
K_1	Carbonaceous deoxygeneration rate constant	day^{-}	0.02-3.4	Yes	Yes
K_2	Reaeration rate constant	day^{-1}	0.0-100	Yes	Yes
K_3	Rate of loss of BOD due to settling	day^{-1}	-0.36-0.36	Yes	Yes
K_4	Benthic oxygen uptake	$\frac{mg\text{-}O}{ft^2\text{-}day}$	Variable	Yes	Yes
K_5	Coliform die-off rate	day^{-1}	0.05-4.0	Yes	Yes
K_5	Arbitrary non-conservative decay coefficient	day^{-1}	Variable	Yes	Yes

TABLE III-3 (cont'd)
TYPICAL RANGES FOR QUAL2E REACTION COEFFICIENTS

Variable	Description	Units	Range of Values	Variable by Reach	Temperature Dependent
β_1	Rate constant for the biological oxidation of NH_3 to NO_2	day^{-1}	0 10-1 00	Yes	Yes
β_2	Rate constant for the biological oxidation of NO_2 to NO_3	day^{-1}	0 20-2 0	Yes	Yes
β_3	Rate constant for the hydrolysis of organic-N to ammonia	day^{-1}	0 02-0 4	Yes	Yes
β_4	Rate constant for the decay of organic-P to dissolved-P	day^{-1}	0 01-0 7	Yes	Yes

4 FUNCTIONAL REPRESENTATION OF TEMPERATURE

4 1 BASIC TEMPERATURE EQUATION

The basic mass transport equation for QUAL2E was given in Section II as (see equation II-3)

$$\frac{\partial C}{\partial t} = \frac{\partial \left(A_x D_L \frac{\partial C}{\partial x}\right)}{A_x \; \partial x} - \frac{\partial (A_x \; \bar{u} \; C)}{A_x \; \partial x} + \frac{dC}{dt} + \frac{s}{V} \qquad \text{IV-1}$$

In temperature modeling, C is taken as the concentration of heat (HL^{-3}) and can be equated to temperature through the relationship

$$C = \rho \; c \; (T - T_0) \qquad \text{IV-2}$$

where

ρ = the density of water ($M \; L^{-3}$)

c = the heat capacity of water ($HM^{-1} \; D^{-1}$)

T = the water temperature

T_0 = an arbitrary base temperature

M = mass

H = heat energy flux

D = degrees

The parameters ρ and c can be considered constant for practical purposes Also, the internal heat generation $\frac{dC}{dt}$, which results from viscous dissipation of energy and boundary friction, is generally small enough to be considered negligible. Thus setting $\frac{dC}{dt} = 0$ in equation IV-1 and substituting equation IV-2 for C gives us (after some simplification)

$$\frac{\partial T}{\partial t} = \frac{\partial(A_x D_L \frac{\partial T}{\partial x})}{A_x \partial x} - \frac{\partial(A_x \bar{u} T)}{A_x \partial x} + \frac{1}{\rho c}\frac{s}{V} \qquad \text{IV-3}$$

The source term s/V (with units of $HL^{-3}T^{-1}$) accounts for all heat transferred across the system boundaries, i.e., heat transferred across the air-water interface and heat conducted across mud-water interface. Heat transfer across the mud-water interface is generally insignificant, hence, s/V takes on the identity of the net rate of heat input per unit volume of stream through the air-water interface.

It is most convenient to represent the interfacial heat transfer rate as a flux (h_N) having units of $HL^{-2}T^{-1}$. For a stream element of length dx and mean surface width W, h_N is related to s/V as follows.

The total rate of heat input across the air-water interface is $h_N\,dx\,W$. This heat is distributed uniformly throughout the underlying volume of $\bar{A}_x\,dx$, where $\bar{A}_x$ is the mean cross-sectional area of the element. Thus the rate of heat gain per unit volume of water, s/V, is computed as

$$\frac{s}{V} = \frac{s}{A_x\,dx} = \frac{h_N\,(W dx)}{\bar{A}_x\,dx} = \frac{h_N}{d} \qquad \text{IV-4}$$

where $d = \bar{A}_x/W$ is the hydraulic depth of the stream. Substituting equation IV-4 into equation IV-3 gives the generalized form of the temperature equation

$$\frac{\partial T}{\partial t} = \frac{\partial(A_x D_L \frac{\partial T}{\partial x})}{A_x \partial x} - \frac{\partial(A_x \bar{u} T)}{A_x \partial x} - \frac{h_N}{\rho c d} \qquad \text{IV-5}$$

4.2 DEFINITION OF h_N

Heat is transferred across the air-water interface of a surface water body by three difference processes: radiation exchange, evaporation, and conduction. The individual heat terms associated with these processes are shown in Figure IV-1 and are defined in Table IV-1 with the typical ranges of their magnitudes in northern latitudes also listed.

The expression that results from the summation of these various energy fluxes is

$$H_N = H_{sn} - H_{an} - (H_b \pm H_c - H_e) \qquad \text{IV-6}$$

where

H_N = net energy flux passing the air-water interface, Btu/ft^2-day

H_{sn} = net short-wave solar radiation flux passing through the interface after losses due to absorption and scattering in the atmosphere and by reflection at the interface, Btu/ft^2-day

H_{an} = net long-wave atmospheric radiation flux passing through the interface after reflection, Btu/ft^2-day

H_b = outgoing long-wave back radiation flux, Btu/ft^2-day

H_c = conductive energy flux passing back and forth between the interface and the atmosphere, Btu/ft^2-day

H_e = energy loss by evaporation, Btu/ft^2-day

These mechanisms by which heat is exchanged between the water surface and the atmosphere are fairly well understood and are adequately documented in the literature by Edinger and Geyer (1965). The functional representation of these terms has been defined by Water Resources Engineers, Inc (1967)

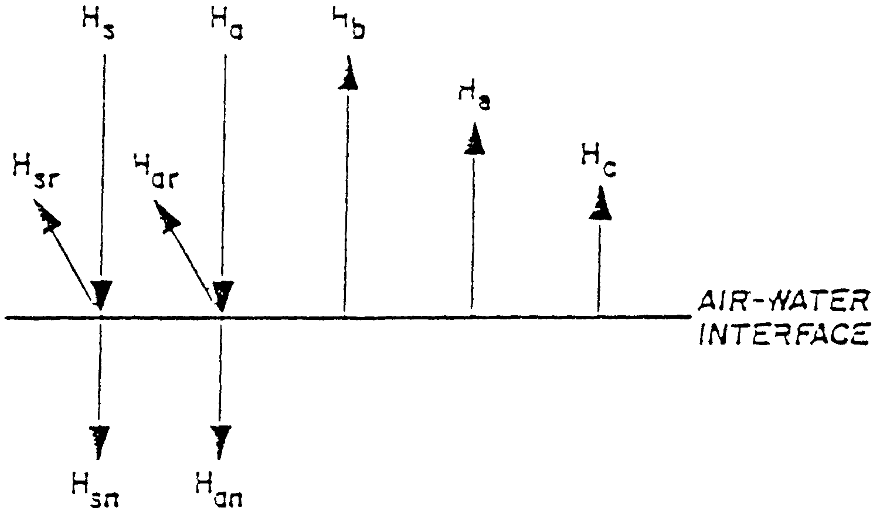


Figure IV-1 Heat Transfer Terms Associated with Interfacial Heat Transfer

TABLE IV-1
DEFINITION OF HEAT TRANSFER TERMS
ILLUSTRATED IN FIGURE 1

		Heat Term	Units	Magnitude ($BTU/ft^2\text{-}day^1$)
H_s	=	total incoming solar or short-wave radiation	$HL^{-2}T^{-1}$	400-2800
H_{sr}	=	reflected short-wave radiation	$HL^{-2}T^{-1}$	40-200
H_a	=	total incoming atmospheric radiation	$HL^{-2}T^{-1}$	2400-3200
H_{ar}	=	reflected atmospheric radiation	$HL^{-2}T^{-1}$	70-120
H_b	=	back radiation from the water surface	$HL^{-2}T^{-1}$	2400-3600
H_e	=	heat loss by evaporation	$HL^{-2}T^{-1}$	150-3000
H_c	=	heat loss by conduction to atmosphere	$HL^{-2}T^{-1}$	-320 to -400

The formulations reported here were extracted from that more detailed work by Frank D. Masch and Associates and the Texas Water Development Board (1971)

4.3 NET SHORT-WAVE SOLAR RADIATION

The net incoming solar radiation is short-wave radiation which passes directly from the sun to the earth's surface. Its magnitude depends on the altitude of the sun, which varies daily as well as seasonally for a fixed location on the earth, the dampening effect of scattering and absorption in the atmosphere due to cloud cover, and the reflection from the water surface

The net amount of solar radiation which reaches the surface of the earth may be represented functionally on an hourly basis by

$$H_{sn} = \underset{(i)}{H_o} \quad \underset{(ii)}{a_t} \quad \underset{(iii)}{(1 - R_s)} \quad \underset{(iv)}{(1 - 0.65C_L^2)} \qquad \text{IV-7}$$

where

H_{sn} = net short-wave solar radiation flux, Btu/ft^2-hr

H_o = amount of radiation flux reaching the earth's atmosphere, Btu/ft^2-hr

a_t = atmospheric transmission term

R_s = Albedo or reflection coefficient

C_L = cloudiness as a fraction of sky covered

It is appropriate for purposes of this discussion to identify and treat separately the four components in equation IV-7 as (i) extraterrestrial solar radiation, (ii) radiation scattering and absorption, (iii) reflectivity, and (iv) cloudiness.

4.3.1 Extraterrestrial Radiation

The short-wave solar radiation flux that strikes the earth's outer atmosphere over a given period of time is given by Water Resources Engineers, Inc. (1967) as

$$H_o = \frac{H_{sc}}{r^2} \left\{ \sin \frac{\pi\phi}{180} \sin \delta \, (t_e - t_b) \right.$$

$$\left. + \frac{12}{\pi} \cos \frac{\pi\phi}{180} \cos \delta \left[\sin \left(\frac{\pi t_e}{12}\right) - \sin \left(\frac{\pi t_b}{12}\right) \right] \right\} \Gamma \qquad \text{IV-8}$$

where

H_{sc} = solar constant = 438.0 Btu/ft^2-hr

r = normalized radius of the earth's orbit

ϕ = latitude of the site, degrees

δ = declination of the sun, degrees

t_b, t_e = hour angles corresponding to the beginning and end, respectively, of any time interval between sunrise and sunset

r = a correction factor for diurnal exposure to radiation flux

Listed below are several parameters in equation IV-8 requiring further definition as described by Water Resources Engineers, Inc (1967)

a Relative Earth-Sun Distance--

$$r = 1.0 + 0.017 \cos \left[\frac{2\pi}{365}(186-Dy)\right] \qquad \text{IV-9}$$

where Dy is the number of the day of the year (beginning January 1)

b Declination--

$$\delta = \frac{23.45}{180} - \cos \left[\frac{2\pi}{365}(173-Dy)\right] \qquad \text{IV-10}$$

c, Hour Angles--

$$t_b = ST_b - \Delta t_s + ET - 12 \qquad \text{IV-11}$$

and

$$t_e = ST_e - \Delta t_s + ET - 12 \qquad \text{IV-12}$$

where ST_b, ST_e are the standard times at the beginning and end of the time interval selected

ET = an expression for time from a solar ephemeris that represents the difference in hours between "true solar time" and that computed on the basis of a yearly average It is given for each day of the year, Dy, by

$$ET = 0.000121 - 0.12319 \sin \left[\frac{2\pi}{365}(Dy-1) - 0.0714\right]$$

$$= 0\ 16549 \sin \left[\frac{4\pi}{365} (Dy-1) + 0\ 3088\right] \qquad \text{IV-13}$$

Δt_s = difference between standard and local civil time in hours as determined from

$$\Delta t_s = \frac{\varepsilon}{15} (L_{sm} - L_{lm}) \qquad \text{IV-14}$$

where

ε = -1 for west longitude

ε = -1 for east longitude

L_{sm} = longitude of standard meridian, degrees

L_{lm} = longitude of local meridian, degrees

d Diurnal Exposure--

$$\Gamma = 1 \text{ when } ST_r \leq ST_b \text{ or } ST_e \leq ST_s \qquad \text{V-15}$$

$$\Gamma = 0 \text{ when } ST_s \leq ST_b \text{ or } ST_e \leq ST_r \qquad \text{IV-16}$$

where ST_r and ST_s are the standard times of sunrise and sunset, respectively, as determined from

$$ST_r = 12 - \frac{12}{\pi} \arccos \left[\tan \left(\frac{\pi\phi}{180}\right) \tan \delta\right] + \Delta t_s \qquad \text{IV-17}$$

and

$$ST_s = 24 - ST_r + 2\Delta t_s \qquad \text{IV-18}$$

4 3 2 Radiation Scattering and Absorption

The atmospheric transmission term, a_t, is given by Water Resources Engineers, Inc (1967) as

$$a_t = \frac{a'' + 0\ 5\ (1 - a' - d)}{1 - 0\ 5\ R_s\ (1 - a' + d)} \qquad \text{IV-19}$$

in which a" is the mean atmospheric transmission coefficient after scattering and absorption, given by

$$a'' = \exp\left\{ -\left[0.465 + 0.0408\, P_{wc}\right] \left[0.179 + 0.421 \exp\left(-0.721\, \theta_{am}\right)\right] \theta_{am}\right\} \qquad \text{IV-20}$$

where θ_{am} is the optical air mass given by the expression

$$\theta_{am} = \frac{\exp(-Z/2531)}{\sin\alpha + 0.15\left(\frac{180\alpha}{\pi} + 3.885\right)^{-1.253}} \qquad \text{IV-21}$$

in which

Z = elevation of the site in feet

α = sun's altitude in radians, given by

$$\alpha = \arcsin\left[\sin\frac{\pi\phi}{180}\sin\delta + \cos\frac{\pi\phi}{180}\cos\delta\cos\frac{\pi t}{12}\right] \qquad \text{IV-22}$$

in which t is the hour angle, described by an equation similar to equation IV-11 and IV-12

P_{wc} in equation IV-20 is the mean daily precipitable water content in the atmosphere, given by the expression

$$P_{wc} = 0.00614 \exp(0.0489 T_d) \qquad \text{IV-23}$$

where T_d is the dewpoint in °F, which can be obtained from the expression

$$T_d = \ln\left[(e_a + 0.0837)/0.1001\right]/0.03 \qquad \text{IV-24}$$

where e_a is the water vapor pressure of the air

The mean atmospheric coefficient, a', can also be represented by an equation of the form of equation IV-20 as

$$a' = \exp\{-[0\ 465 + 0\ 0408\ P_{wc}]\ [0\ 129 + 0\ 171 \exp(-0\ 980\ \theta_{am})]\ \theta_{am}\} \qquad \text{IV-25}$$

Dust attenuation of the solar radiation flux, which is represented in equation IV-19 by the quantity d, varies with optical air mass, season of the year, and geographic location Water Resources Engineers, Inc (1967) gives a range of 0-0 13 for several locations

4 3 3 Cloudiness

The dampening effect on the solar radiation flux is given by Water Resources Engineers, Inc (1967) as

$$C_s = 1\ 0 - 0\ 65\ C_L^2 \qquad \text{IV-26}$$

where C_L is the decimal fraction of the sky covered Water Resources Engineers, Inc (1967) reports that equation IV-26 gives satisfactory results except for heavy overcast conditions, i e , when C_L approaches 1 0

4 3 4 Reflectivity

The reflection coefficient, R_s, can be approximately computed as a function of the solar altitude, α, by Anderson's (1954) empirical formula

$$R_s = A\alpha^B \qquad \text{IV-27}$$

where α is in degrees, and A and B are functions of cloudiness, C_L Values for A and B given by Anderson (1954) are shown in Table IV-2

TABLE IV-2
EMPIRICAL COEFFICIENTS FOR DETERMINING R_s
After Anderson (1954)

Cloudiness C_L	0 Clear		0 1 - 0 5 Scattered		0 6 - 0 9 Broken		1 0 Overcast	
Coefficients	A	B	A	B	A	B	A	B
	1 18	-0 77	2 20	-0 97	0 95	-0 75	0 35	-0 45

15

4.4 LONG-WAVE ATMOSPHERIC RADIATION

The long-wave radiation emitted by the atmosphere varies directly with the moisture content of the atmosphere. Although it is primarily dependent on air temperature and humidity, it can also be affected by ozone, carbon dioxide, and possibly other materials in the atmosphere. Anderson (1954) indicated that the amount of atmospheric radiation is also significantly affected by cloud height. The amount of long-wave atmospheric radiation that is reflected is approximately a constant fraction of the incoming radiation, found by Anderson (1954) to be approximately 0.03.

The net atmospheric radiation flux can be expressed as

$$H_{an} = [2.89 \times 10^{-6}]\ \sigma\ (T_a + 460)^6\ (1.0 - 0.17C_L^2)(1-R_L) \qquad \text{IV-28}$$

where

H_{an} = net long-wave atmospheric radiation flux, Btu/ft^2-hr

σ = Stefan-Boltzman constant, 1.73 x 10^{-9} Btu/ft^2/hr/°Rankine^4

T_a = air temperature at a level 6 feet above the water surface, °F

R_L = reflectivity of the water surface for atmospheric radiation = 0.03

C_L = cloudiness, fraction of cloud cover

4.5 WATER SURFACE BACK RADIATION

The third source of radiation transfer through the air-water interface is long-wave back radiation from the water surface, H_b, which represents a loss of heat from the water. It can be seen from Table IV-1 that back radiation accounts for a substantial portion of the heat loss from a body of water. This loss is expressed by the Stefan-Boltzman Fourth Power Radiation Law for a blackbody as

$$h_b = 0.97\ \sigma\ (T_s + 460)^4 \qquad \text{IV-29}$$

where

h_b = water surface back radiation flux, Btu/ft^2-hr

T_s = water surface temperature, °F

Equation IV-29 can be linearized over a given temperature range as

$$H_b = \alpha_2 - \beta_2 T_s \qquad \text{IV-30}$$

where

α_2, β_2 = constants defined over the range 35 to 135 °F

In the steady-state temperature solution, this linearized version of the back radiation equation is used to allow the temperature dependent terms to be separated out of the equation Sets of α_2, β_2 are specified for 21 5°F temperature intervals between 35°F and 135°F For dynamic simulations the heat flux term calculations are based on the temperature at the beginning of the time step

4 6 EVAPORATION

A water body also loses heat to the atmosphere by evaporation Each pound of water that leaves as water vapor carries its latent heat of vaporization (approximately 1050 BTU at 60°F) plus its sensible heat This significant heat loss due to evaporation can be expressed as

$$H_e = \gamma H_L E + H_v \qquad \text{IV-31}$$

where

γ = specific weight of the water being evaporated, lb/ft^3

H_L = latent heat of vaporization, Btu/lb, given by

H_L = $1084 - 0.5\ T_s$

E = evaporation rate, ft/hr

H_v = sensible heat loss Btu/ft^2-hr

The evaporation rate, E, is most often expressed as

$$E = (a + bW)\ (e_s - e_a) \qquad \text{IV-32}$$

where

a,b = constants

W = wind speed, in mph measured 6 feet above the water surface

e_s = saturation vapor pressure of the air, in of Hg, at the temperature of the water surface, as given by

e_s = $0\ 1001 \exp (0\ 03\ T_s) - 0\ 0837$

and

e_a = water vapor pressure, in of Hg, at a height of 6 feet above the water surface, given as

$$e_a = e_{wb} - 0\ 000367\ P_a\ (T_a - T_{wb}) \left(1\ 0 - \frac{T_{wb} - 32}{1571}\right) \qquad \text{IV-34}$$

where

e_{wb} = saturation vapor pressure, in of Hg, at the wet bulb temperature from the expression

$$e_{wb} = 0\ 1001 \exp (0\ 03\ T_{wb}) - 0\ 0837 \qquad \text{IV-35}$$

P_a = local barometric pressure, in of Hg

T_{wb} = wet bulb air temperature, °F

T_a = dry bulb air temperature, °F

The literature contains a wide range of values for the evaporation constants a and b Roesner (1969) reports that a good average value of a would be 6 8 x 10^{-4} ft/hr-in of Hg, while b would best be represented by 2 7 x 10^{-4} ft/hr-in of Hg -mph

To linearize the variation of evaporation rate with surface water temperature T_s, equation IV-34 is approximated over 5°F intervals as

$$e_s = \alpha_1 - \beta_1 T_s \qquad \text{IV-36}$$

Sets of α_1, β_1 are specified for twenty-one 5°F intervals between 35°F and 135°F The linearized evaporation expression is used in the steady-state temperature solution

The sensible evaporative heat loss can be expressed simply as

$$H_v = c \gamma E (T_s - T_0) \qquad \text{IV-37}$$

where

c = heat capacity of water = 1 Btu/lb-°F

T_0 = reference temperature, °F

Sensible heat loss is very small compared to the other heat loss components in the energy budget and thus is not included in the QUAL2E temperature computation.

4.7 CONDUCTION

Heat that is transferred between the water and the atmosphere due to a temperature difference between the two phases and not related to water vapor exchange is normally called conduction. Using the fact that transfer by conduction is a function of the same variables as evaporation, it is possible to arrive at a proportionality between heat conduction and heat loss by evaporation. This proportionality, known as Bowen's ratio, is expressed as

$$B = \frac{H_c}{H_e} = C_B \left[\frac{T_s - T_a}{e_s - e_a}\right] \frac{P_a}{29.92} \qquad \text{IV-38}$$

where C_B is a coefficient $\equiv 0.01$

By using Bowen's ratio, the rate of heat loss to the atmosphere by heat conduction, H_c, can be defined as

$$H_c = \gamma H_L (a+bW) \left(0.01 \frac{P_a}{29.92}\right) (T_s - T_a) \qquad \text{IV-39}$$

For practical purposes, the ratio ($P_a/29.92$) can be taken as unity.

4.8 QUAL2E MODIFICATIONS FOR REACH VARIABLE LOCAL CLIMATOLOGY AND TEMPERATURE

Prior versions of QUAL-II and QUAL2E have assumed that the input variables for temperature simulation were uniform over the entire river basin (global inputs). These input variables consist of climatological, geographical, and heat balance information as follows: basin elevation, dust attenuation coefficient, evaporation coefficients, dry and wet bulb air temperatures, atmospheric pressure, cloud cover, and wind speed. In the current version of QUAL2E most of these inputs, with the exception of the evaporation coefficients are reach variable. Thus, for systems in which variable ambient temperature and climatology may be important, for example in modeling rivers with large changes in elevation, different values for these factors may be supplied for each reach in the river. The overall heat balance computations are performed as described in Sections 4.1-4.7 of this chapter, using the reach specific values of each input variable. When reach variable temperature simulation inputs are used, a detailed temperature and heat balance summary is provided with the QUAL2E final output.

The user has a number of options in specifying the input variables for temperature simulation. Global values may be used (all reaches having the same values for each of the temperature simulation inputs), or different input values may be explicitly specified for each reach in the system. In the case where reach specific values of atmospheric pressure are not known or available, QUAL2E has the capability of estimating the value of atmospheric pressure for each reach from its elevation and air temperature. These estimates are computed from the ideal gas law integrated over the change in elevation relative to a datum (Plate, 1982)

$$P = P_0 \; e^{[-(g/RT)(z - z_0)]} \qquad \text{IV-40}$$

Where

P = atmospheric pressure at elevation z (in Hg),

g = gravitational constant (32.2 ft/sec^2),

R = gas law constant (1715 ft^2/sec^2-$^{\circ}$R),

T = dry bulb air temperature ($^{\circ}$R),

z = elevation of reach (ft),

z_0, P_0 = datum elevation and pressure, respectively,

The principal assumptions used in deriving Eq. IV-40 are that air temperature and specific humidity are constant. Thus, the value of the gas constant, R, is that for dry air and the value of dry bulb air temperature, T, is the average of the dry bulb temperatures at elevations z and z_0. Although refinements to this methodology are possible, they were deemed premature until more experience with this option is obtained. If the reach variable values of atmospheric pressure are computed from Eq. IV-40, they are echo-printed with the QUAL2E output.

5 COMPUTATIONAL REPRESENTATION

5 1 PROTOTYPE REPRESENTATION

To expand upon the basic conceptual representation presented in Sections 1 and 2, QUAL2E permits any branching, one-dimensional stream system to be simulated The first step involved in approximating the prototype is to subdivide the stream system into reaches, which are stretches of stream that have uniform hydraulic characteristics Each reach is then divided into computational elements of equal length so that all computational elements in all reaches are the same length Thus, all reaches must consist of an integer number of computational elements

There are seven different types of computational elements

1 Headwater element

2 Standard element

3 Element just upstream from a junction

4 Junction element

5 Last element in system

6 Input element

7 Withdrawal element

Headwater elements begin every tributary as well as the main river system, and as such, they must always be the first element in a headwater reach A standard element is one that does not qualify as one of the remaining six element types Because incremental flow is permitted in all element types, the only input permitted in a standard element is incremental flow A type 3 element is used to designate an element on the mainstem that is just upstream of a junction A junction element (type 4), has a simulated tributary entering it Element type 5 identifies the last computational element in the river system (downstream boundary), there should be only one element type 5 Element types 6 and 7 represent elements which have inputs (waste loads and unsimulated tributaries) and water withdrawals, respectively

River reaches, which are aggregates of computational elements, are the basis of most data input. Hydraulic data, reaction rate coefficients, init conditions, and incremental flow data are constant for all computational elements within a reach.

5.2 FORCING FUNCTIONS

Forcing functions are the user specified inputs that drive the system being modeled. These inputs are specified in terms of flow, water quality characteristics, and local climatology. QUAL2E accommodates four types of hydraulic and mass load forcing functions in addition to local climatological factors--headwater inputs, point sources or withdrawals, incremental inflow/outflow along a reach, and the (optional) downstream boundary concentration.

1. Headwater Inputs - Headwater inputs are typically the upstream boundary conditions at the beginning of the system. They are the conditions required to generate the solution of the mass balance equations for the first computational element in each headwater reach. Headwaters are also the source of water for flow augmentation.

2. Point Sources and/or Withdrawals - These loads are used to represent point source discharges into the system (i.e., sewage and industrial waste, or storm water runoff) and losses from the system resulting from diversions. In QUAL2E point source discharges may represent either raw or treated waste loads. If raw waste loads are used, the effect of treatment can be simulated by applying a specific fractional removal for carbonaceous BOD to each point source load.

3. Incremental Inflow - QUAL2E has the capability to handle flow uniformly added or removed along a reach. The total flow increment along a reach is apportioned equally to all computational elements in the reach. This feature can be used to simulate the effects of non-point source inputs to the system, or the effect of loss of stream flow to the groundwater.

4. Downstream Boundary Concentration (optional) - QUAL2E has the capability of incorporating known downstream boundary concentrations of the water quality constituents into the solution algorithm. This feature is useful in modeling systems with large dispersion in the lower reaches (e.g., estuaries). When downstream boundary concentrations are supplied, the solution generated by QUAL2E will be constrained by this boundary condition. If the concentrations are not provided, the constituent concentrations in the most downstream element will be computed in the normal fashion using the zero gradient assumption (see Section 5.4.3).

Local climatological data are required for the simulation of algae and temperature. The temperature simulation uses a heat balance across the air-water interface and thus requires values of wet and dry bulb air temperatures, atmospheric pressure, wind velocity, and cloud cover. The algal simulation requires values of net solar radiation. For dynamic simulations, these climatological data must be input at regular time intervals over the course of the simulation and are applied uniformly over the entire river basin For modeling steady-state temperature and algae, average daily local climatological data are required and may vary spatially over the basin by reach

5 3 MODEL LIMITATIONS

QUAL2E has been developed to be a relatively general program, however, certain dimensional limitations have been imposed upon it during program development These limitations are as follows

Reaches a maximum of 25

Computational elements no more than 20 per reach or 250 in total

Headwater elements a maximum of 7

Junction elements a maximum of 6

Input and withdrawal elements a maximum of 25 in total

(Note These limitations may be modified, if necessary, by the user by altering the PARAMETER statement specifications in file MAIN VAR of the program and recompiling

QUAL2E can be used to simulate any combination of the following parameters or groups of parameters

1 Conservative minerals (up to three at a time)

2 Temperature

3 BOD

4 Chlorophyll a

5 Phosphorus cycle (organic and dissolved)

6 Nitrogen cycle (organic, ammonia, nitrite, and nitrate)

7 Dissolved oxygen

8 Coliforms

9 An arbitrary nonconservative constituent

All parameters can be simulated under either steady-state or dynamic conditions If either the phosphorus cycle or the nitrogen cycle are not being simulated, the model presumes they will not limit algal growth

5.4 Numerical Solution Technique

At each time step and for each constituent, Equation II-3 can be written I times, once for each of the I computational elements in the network. Because it is not possible to obtain analytical solutions to these equations under most prototype situations, a finite difference method is used--more specifically, the classical implicit backward difference method (Arden and Astill, 1970, Smith, 1966, and Stone and Brian, 1963).

The general basis of a finite difference scheme is to find the value of a variable (e.g., constituent concentration) as a function of space at a time step $n+1$ when its spatial distribution at the n^{th} time step is known. Time step zero corresponds to the initial condition. Backward difference or implicit schemes are characterized by the fact that all spatial derivatives ($\partial/\partial x$) are approximated in difference form at time step $n-1$.

5.4.1 Formulation of the Finite Difference Scheme

The finite difference scheme is formulated by considering the constituent concentration, C, at four points in the mnemonic scheme as shown in Figure V-1.

Three points are required at time $n-1$ to approximate the spatial derivatives. The temporal derivative is approximated at distance step i.

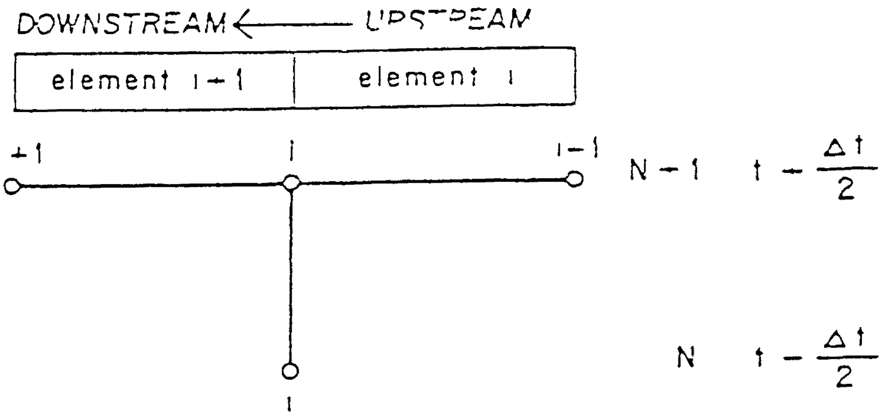


Figure V-1 Classical Implicit Nodal Scheme

Equation II-3 can be written in finite difference form in two steps First, the advection and diffusion terms are differentiated once with respect to x, giving

$$\frac{\partial C_i}{\partial t} = \frac{\left(AD_L \dfrac{\partial C}{\partial x}\right)_i - \left(AD_L \dfrac{\partial C}{\partial x}\right)_{i-1}}{V_i} - \frac{(A\,\bar{u}\,C)_i - (A\,\bar{u}\,C)_{i-1}}{V_i}$$

$$+ \frac{dC_i}{dt} - \frac{s_i}{V_i} \qquad \text{V-1}$$

where

$$V_i = A_i \, \Delta x_i$$

Secondly, expressing the spatial derivative of the diffusion terms in finite difference and thence the time derivative of C in finite difference, there results

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \left(\frac{[(AD_L)_i]\, C_{i+1}^{n+1} - [(AD_L)_i]\, C_i^{n+1}}{V_i \, \Delta x_i}\right.$$

$$\left. - \frac{[(AD_L)_{i-1}]\, C_i^{n+1} - [(AD_L)_{i-1}]\, C_{i+1}^{n+1}}{V_i \, \Delta x_i}\right)$$

$$- \left(\frac{Q_i\, C_i^{n+1} - Q_{i-1}\, C_{i+1}^{n+1}}{V_i}\right) + r_i\, C_i^{n+1} + p_i - \frac{s_i}{V_i} \qquad \text{V-2}$$

In equation V-2, the term dC/dt is expressed as

$$\frac{dC_i}{dt} = r_i\, C_i^{n+1} + p_i$$

where

r = first order rate constant

p_i = internal constituent sources and sinks (e g , nutrient loss from algal growth, benthos sources, etc)

Note that the dC/dt for every constituent modeled by QUAL2E can be expressed in this form.

If equation V-2 is rearranged in terms of the coefficients of C_{i-1}^{n+1}, C_i^{n+1}, and C_{i+1}^{n+1}, we obtain the equation

$$a_i \, C_{i-1}^{n+1} - b_i \, C_i^{n+1} + c_i \, C_{i+1}^{n+1} = Z_i \qquad \text{V-3}$$

where

$$a_i = - \left[(AD_L)_{i-1} \frac{\Delta t}{V_i \, \Delta x_i} - \frac{Q_{i-1} \, \Delta t}{V_i} \right]$$

$$b_i = 1.0 - \left[(AD_L)_i - (AD_L)_{i-1} \right] \frac{\Delta t}{V_i \, \Delta x_i} + Q_i \frac{\Delta t}{V_i} - r_i \, \Delta t$$

$$c_i = - \left[(AD_L)_i \frac{\Delta t}{V_i \, \Delta x_i} \right]$$

$$Z_i = C_i^{\,n} - \frac{s_i \, \Delta t}{V_i} + p_i \, \Delta t$$

The values of a_i, b_i, c_i, and Z_i are all known at time n, and the C_i^{n+1} terms are the unknowns at time step n+1.

In the case of a junction element with a tributary upstream element, the basic equation becomes

$$a_i \, C_{i-1}^{n+1} - b_i \, C_i^{n+1} - c_i \, C_{i+1}^{n+1} + d_j \, C_j^{n+1} = Z_i \qquad \text{V-4}$$

where

$$d_j = - \left[(AD)_j \frac{\Delta t}{V_i \, \Delta x_i} - \frac{Q_j \, \Delta t}{V_i} \right]$$

j = the element upstream of junction element i

C_j^{n+1} = concentration of constituent in element j at time n+1

It can be seen that the d_j term is analogous to the a_i term. Both terms account for mass inputs from upstream due to dispersion and advection.

Under steady-state conditions, $\frac{\partial C_i}{\partial t} = 0$ in equation V-1. Working through the finite difference approximations and rearranging terms as before, the steady-state version of equation V-3 is derived

$$a_i\ C^{n+1}_{i-1} - b_i\ C^{n+1}_{i} + c_i\ C^{n+1}_{i+1} = Z_i \qquad \text{V-5}$$

where

$$a_i = -\left[\frac{(AD_L)_{i-1}}{V_i \Delta x_i} + \frac{Q_{i-1}}{V_i}\right]$$

$$b_i = \left[\frac{(AD_L)_i}{V_i \Delta x_i} - \frac{(AD_L)_{i-1}}{V_i \Delta x_i} - \frac{Q_i}{V_i} - r_i\right]$$

$$c_i = \left[\frac{(AD_L)_i}{V_i \Delta x_i}\right]$$

$$Z_i = \frac{S_i}{V_i} + P_i$$

Note that equation V-5 is the same as equation V-3, with three changes

- $\Delta t = 1.0$
- the constant 1.0 in $b_i = 0.0$
- the initial concentration C^n_i in $Z_i = 0.0$

5.4.2 Method of Solution

Equations V-3 and V-5 each represent a set of simultaneous linear equations whose solution provides the values of C^{n+1}_i for all i's. Expressed in matrix form, this set of equations appears as

$$\begin{bmatrix} b_1 & c_1 & & & & & \\ a_2 & b_2 & c_2 & & & & \\ & a_3 & b_3 & c_3 & & & \\ & & & & & & \\ & & a_i & b_i & c_i & & \\ & & & & & & \\ & & & & a_{I-1} & b_{I-1} & c_{I-1} \\ & & & & & a_I & b_I \end{bmatrix} \times \begin{bmatrix} C_1^{n+1} \\ C_2^{n+1} \\ C_3^{n+1} \\ \\ C_i^{n+1} \\ \\ C_{I-1}^{n+1} \\ C_I^{n+1} \end{bmatrix} = \begin{bmatrix} Z_1 \\ Z_2 \\ Z_3 \\ \\ Z_i \\ \\ Z_{I-1} \\ Z_I \end{bmatrix} \qquad \text{V-6}$$

The left matrix is a tri-diagonal matrix. An efficient method that readily lends itself to a computer solution of such a set of equations is

Divide through the first equation in V-6 by b_1 to obtain

$$C_1^{n+1} - W_1 C_2^{n-1} = G_1 \qquad \text{V-7}$$

where

$$W_1 = c_1/b_1 \text{ and } G_1 = Z_1/b_1$$

Combine the expression for b_1 (see V-3) and the second equation in V-6 to eliminate a_2 and the result is

$$C_2^{n+1} + W_2 C_3^{n-1} = G_2 \qquad \text{V-8}$$

where

$$W_2 = \frac{c_2}{b_2 - a_2 W_1} \text{ and } G_2 = \frac{Z_2 - a_2 G_1}{b_2 - a_2 W_1}$$

Combine equation V-8 and the third equation in V-6 to eliminate a_3 and the result is

$$C_3^{n+1} + W_3\, C_4^{n+1} = G_3 \qquad \text{V-9}$$

where

$$W_3 = \frac{c_3}{b_3 - a_3 W_2} \quad \text{and} \quad G_3 = \frac{Z_3 - a_3 G_2}{b_3 - a_3 W_2}$$

Proceed through the equations, eliminating a_i and storing the values of W_i and G_i given by

$$W_i = \frac{c_i}{b_i - a_i W_{i-1}}, \quad i = 2, 3, \ldots, I \qquad \text{V-10}$$

and

$$G_i = \frac{Z_i - a_i G_{i-1}}{b_i - a_i W_{i-1}}, \quad i = 2, 3, \ldots, I \qquad \text{V-11}$$

The last equation is solved for C_I^{n+1} by

$$C_I^{n+1} = G_I \qquad \text{V-12}$$

Solve for C_{I-1}^{n+1}, C_{I-2}^{n+1}, …, C_1^{n+1} by back substitution

$$C_i^{n+1} = G_i - W_i\, C_{i-1}^{n+1}, \quad i = I-1, I-2, \ldots, 1 \qquad \text{V-13}$$

5.4.3 Boundary Conditions

In most situations of interest, transport is unidirectional in nature i.e., there is no significant transport upstream. Therefore, the concentration at some point just upstream from the beginning or end of the stream reach of interest can be used as the boundary condition.

5.4.3.1 Upstream Boundary (Headwater Elements)

For headwater elements there is no upstream, i-1, element. Thus, the headwater driving force is substituted in Equation V-3 for the upstream concentration C_{i-1}. Because the headwater concentrations are fixed, they are incorporated on the right hand side of Equation V-3 in the known term Z_i, for headwater elements as follows

$$Z_1 = C_1^n + \frac{s_1 \Delta t}{V_1} + p_1\, \Delta t - a_1\, C_0 \qquad \text{V-14}$$

where C_0 is the upstream boundary condition (headwater concentration)

5.4.3.2 Downstream Boundary (Last Element in the System)

QUAL2E has two options for modeling the downstream boundary. One uses zero gradient assumption, the other incorporates fixed downstream constituent concentrations into the solution algorithm.

Zero Gradient Assumption (Arden and Astill, 1970)--For the last computational element in the system, there is no downstream, i+1, element. At this boundary, a zero gradient assumption is made that replaces C_{i+1} with C_{i-1}. In this manner, the downstream boundary acts as a mirror to produce a zero gradient for the concentration of the constituent variable. The coefficient a_i, therefore, is modified to include the dispersion effect normally found in the coefficient c_i for the last element in the system. Thus, the equation for a_i in V-3 becomes

$$a_I = -[((AD_L)_{I-1} + (AD_L)_I) \frac{\Delta t}{V_I \Delta x_I} + \frac{Q_{I-1}\Delta t}{V_I}] \qquad \text{V-15}$$

and

$$c_I = 0 \qquad \text{V-16}$$

where I = index of the downstream boundary element

Fixed Downstream Constituent Concentrations--For this boundary option, the user supplies known downstream boundary concentrations C_{LB} for each water quality constituent. Thus, the value of C_{i+1} in Equation V-3 becomes

$$C_{i+1} = C_{LB} \qquad \text{V-17}$$

Because the boundary concentrations are known in this option, they are incorporated on the right hand side of Equation V-3 in the known term Z_i for the downstream boundary element then results as

$$Z_I = C_I^n + \frac{s_I \Delta t}{V_I} + p_I \Delta t - c_I C_{LB} \qquad \text{V-18}$$

6 UNCERTAINTY ANALYSIS WITH QUAL2E

6 1 INTRODUCTION

Uncertainty analysis for model simulations is assuming a growing importance in the field of water quality management The impetus for this concern is provided by recent public awareness over health risks from improper disposal of toxic wastes as well as by the continuing emphasis within EPA on risk assessment One of the first steps in the chain of risk assessment is the quantification of the error in predicting water quality Unfortunately, uncertainty analysis of water quality model forecasts has not received as much attention in practice as has the prediction of expected (average) values

Uncertainty analysis has been the subject of much discussion in the ecosystem modeling literature (Rose and Swartzman, 1981 and O'Neill and Gardner, 1979) In the water resources literature, lake eutrophication models have been used to compare various methods of uncertainty analysis (Reckhow, 1979, Scavia et al , 1981, and Malone et al , 1983) The methodologies described in this chapter represent a systematic approach to uncertainty analysis for the general purpose stream water quality model QUAL2E The objective is to provide some of the tools for incorporating uncertainty analysis as an integral part of the water quality modeling process The QUAL2E model was chosen for this application because it is a general purpose computer code, widely used by consultants and state regulatory agencies in waste load allocation and other planning activities The resulting uncertainty model is named QUAL2E-UNCAS

6 2 QUAL2E-UNCAS

Three uncertainty analysis techniques can be employed in QUAL2E-UNCAS--sensitivity analysis, first order error analysis, or monte carlo simulation The user is provided this array of options for flexibility, because the methods differ in their assumptions and will not always agree with each other Discrepancies may be explained by errors in the first order approximation or by errors due to biased variance calculations Monte carlo simulation has the advantage of output frequency distributions, but it carries a high computational burden First order error propagation provides a direct estimate of model sensitivity, but that variability is usually more indicative of the variance of model components than of the dynamics of the model structure

The methodology provided in QUAL2E-UNCAS allows the model user to perform uncertainty analysis with relative ease and efficiently manages the output from the analysis Although the application is specific to the QUAL2 model, the methodology is general The preprocessing and postprocessing algorithms used are, in principle, applicable to many water quality models The preprocessor allows the user to select the variables and/or parameters to be altered, without having to manually restructure the input data set This task is performed automatically by the preprocessor for as many uncertainty conditions as the user wishes to simulate The postprocessor stores and manipulates only the output of interest, thus reducing potential voluminous output The user must select the important variables and locations in the stream network where uncertainty effects are desired for analysis

6 2 1 Sensitivity Analysis

In normal usage sensitivity analysis is accomplished using a one-variable-at-a-time approach (Duke, 1976) Sensitizing more than one input variable at a time is an attractive method for assessing their interaction effects on the output variable When many input parameters and variables ar altered, however, the number of combinations to be investigated becomes large, thus complicating interpretation of the results Experimental design strategies can be efficiently applied in this situation to elicit main and interaction effects of input variables

With the sensitivity analysis option in QUAL2E-UNCAS, the user may vary the inputs singly, in groups, or using factorial design strategies The input requirements for sensitivity analysis consist of identifying the input variables to be perturbed and specifying the magnitude of the perturbation The output for each sensitivity simulation consists of the changes (i e , th sensitivities) in the value(s) of each output variable (ΔY) resulting from the changes in the value(s) of the input variables (ΔX) This output is provided in tabular format, similar to the QUAL2E final summary, except that the table entries are sensitivities rather than the values of the output variables

QUAL2E-UNCAS also has the capability of assessing the main and interaction effects of input variables on various output variables by sensitizing the inputs according to 2-level factorial design strategies Currently QUAL2E-UNCAS accommodates only 2-variable (i e , 2^2) and 3-variable (i e , 2^3) factorial designs As in normal sensitivity analysis, the user specifies the names of the input variables to be perturbed and the magnitude of the perturbation The factorial design computations for main and interaction effects are performed using standard statistical procedures (Box et al , 1978, and Davies, 1967)

Because QUAL2E computes values of each output variable for every computational element in the system, the factorial design output would be voluminous if performed for each element Thus, the user must specify particular locations (maximum of 5) in the basin where this analysis is to be performed The critical locations, such as the dissolved oxygen sag point, or the location below the mixing zone of a tributary junction or point discharge, are usually included among those chosen for analysis

6 2 2 First Order Error Analysis

First order error analysis utilizes the first order approximation to the relationship for computing variances in multivariate situations The input variables are assumed to act independently (covariances are ignored) and the model to be linear (the higher order terms of the Taylor expansion are omitted) The first order approximations to the components of output variance is often good (Walker, 1982)

The QUAL2E-UNCAS output for first order error analysis consists of two parts--(a) a tabulation of normalized sensitivity coefficients and (b) a listing of the components of variance The normalized sensitivity coefficients represent the percentage change in the output variable resulting from a 1 percent change in each input variable, and are computed as follows

$$S_{ij} = (\Delta Y_j/Y_j)/(\Delta X_i/X_i) \qquad \text{VI-1}$$

where

S_{ij} = normalized sensitivity coefficient for output Y_j to input X_i,

X_i = base value of input variable,

ΔX_i = magnitude of input perturbation,

Y_j = base value of output variable,

ΔY_j = sensitivity of output variable

The components of variance for each output variable Y are the percentages of output variance attributable to each input variable X, computed in the following manner

$$Var(Y_j) = \sum_i Var(X_i)(\Delta Y_j/\Delta X_i)^2 \qquad \text{VI-2}$$

where

$Var(Y_j)$ = variance of output variable Y_j,

$Var(X_i)$ = variance of input variable X_i,

Y_j and X_i are as defined in Eq VI-1

As can be seen from Eq V-2, each term in the summation is a component of the variance of the output variable, Y_j, contributed by the input variabl X_i. The components of the output variance, Var(Y_j), represent a weighting o the input variances, Var(X_i), by the square of the sensitivity of model outp to input, ($\Delta Y_j/\Delta X_i$). Thus, a particular input variable may be a large (smal contributor to the output variance if it has either a large (small) input variance or a large (small) sensitivity coefficient, or both. Performing multiple first order error analyses with differing values of X_i will provide an estimate of the strength of model nonlinearities. Outputs that are linea in X_i will have unchanging sensitivity coefficients, ($\Delta Y_j/\Delta X_i$), as ΔX_i chang

In normal applications of first order error analysis, all of the input variables are perturbed. In this manner, the contributions to output varianc from all input variables are computed. QUAL2E-UNCAS has the capability, however, of constraining the number of input variables to be included in a first order analysis. This limitation is achieved by allowing the user to specify the generic group of inputs (i.e., "hydraulic variables," "reaction coefficients," "point load forcing functions," etc.) that are to be perturbe in the analysis.

The input requirements for first order error analysis consist of (a) the magnitude of the input perturbation, ΔX_i, and (b) the value of the variance of the input variable, Var(X_i). The value of ΔX_i (default value is 5%, i.e., $\Delta X_i/X_i$ = 0.05) is specified by the user and applied uniformly over all inputs for the purpose of computing sensitivities. Default values for the input variances are provided with the QUAL2E-UNCAS model (see Section 6.3); however, users are cautioned to use values appropriate to their modeling application. Finally, as in the factorial design option, the user must choose the locations (maximum of 5) in the basin at which the first order error analysis for the output variables is to be performed.

6.2.3 Monte Carlo Simulation

Monte carlo simulation is a method for numerically operating a complex system that has random components. Input variables are sampled at random from pre-determined probability distributions (with or without correlation) and the distribution of output values from repeated simulations is analyzed statistically. The validity of this method is not affected by nonlinearities in the water quality model.

The monte carlo simulation computations in QUAL2E-UNCAS provide summary statistics and frequency distributions for the state variables at specific locations in the system. The summary statistics include: mean (base and simulated), bias, minimum, maximum, range, standard deviation, coefficient of variation, and skew coefficient. Frequency and cumulative frequency distributions are tabulated in increments of one-half a standard deviation. Comparison of the standard deviation estimates from monte carlo simulations with those from first order error analysis provide an indication of the extent of model nonlinearities. Cumulative frequency distributions are useful in evaluating overall dispersion in the model predictions and in assessing the likelihood of violating a water quality standard.

The input requirements for the monte carlo simulation option in QUAL2E-UNCAS consist of (a) the variance of the input variable, $Var(X_i)$, (b) the probability density function of the input variable, and (c) the number of simulations to be performed Specification of input variances is done in the same manner as that for first order error analysis Currently there are two options for the input probability density functions normal and log-normal The distribution for each input variable can be specified from either of these options The default option is the normal distribution The number of monte carlo simulations must be large enough to avoid large errors in the estimated values of output variance, yet small enough to avoid unduly long computation times Preliminary experience with UNCAS indicates that about 2000 simulations are required to achieve estimates of output standard deviations with 95% confidence intervals of 5%

QUAL2E-UNCAS assumes that all inputs act independently Thus, each input is randomized independently from the others In normal usage, all input variables are randomized in monte carlo simulation As in the case of first order error analysis, however, the user may constrain the number of inputs to be varied by specifying that only certain generic groups of inputs be randomized Lastly, the user must specify the locations (maximum of five) in the basin at which monte carlo simulation results are to be tabulated

6 3 Input Variable Variances

One of the fundamental requirements for performing uncertainty analyses in water quality modeling is a knowledge of the uncertainty characteristics of the model inputs Information on model input uncertainty is not widely available in the literature, although recent articles show an increasing tendency to publish such information (Kennedy and Bell, 1986) Three reports (Koenig, 1986, NCASI, 1982, and McCutcheon, 1985) have been examined to compile an uncertainty data base for use with QUAL2E-UNCAS A summary of this information is shown in Table VI-1 These values represent ranges in the uncertainty of model inputs caused by such factors as spatial variation, temporal variation, sampling error, analytical error, and bias in measurement or estimation technique

In QUAL2E-UNCAS, uncertainty information is provided in two forms (a) the value of the variance of the input variables and (b) the specification of a probability density function for each input. The model reads this information, as required, from a data file named "INVAR DAT " An example of this file, containing a set of default values for all QUAL2E inputs, is provided with the QUAL2E-UNCAS model These data are consistent with the typical ranges of uncertainty shown in Table VI-1 and are provided only as a guide for beginning the process of estimating the uncertainty associated with QUAL2E input variables All users are CAUTIONED not to assume that these values are appropriate to all modeling situations The burden of verifying and confirming input variance estimates for a particular application lies with the user Efforts to develop a better understanding of input variable uncertainties are continuing

TABLE VI-1
SUMMARY OF QUAL2E INPUT VARIABLE UNCERTAINTIES

Input Variable or Parameter	QUAL2E Data Type	Relative Standard Deviation, Low	Typical	High
Algae, Nutrient, Light Coefficients	1A	5	10-20	50
Temperature Coefficients	1B	1	2-5	10
Hydraulic Data	5	1	5-15	50
Temperature/LCD	5A	1	2-10	20
Reaction Coefficients	6	5	10-25	100
Constituent Concentrations	8,10,11			
Temperature		1	2-3	5
DO		2	5-10	15
CBOD		5	10-20	40
N Forms		10	15-30	75
P Forms		10	15-40	75
Algae		5	10-25	50
Coliform		20	25-50	100
Conservative Minerals		1	5-10	15

Summary of data compiled from APHA, 1985, Koenig, 1986, McCutcheon, 1985, and NCASI, 1982a

In the general case, QUAL2E-UNCAS accepts input variability information in relative rather than absolute units Thus, the input perturbations for first order error analysis and input variances for first order analysis and monte carlo simulation are supplied as percent perturbation and coefficient of variation, respectively The transformation equations between relative and absolute units are

$$\Delta X_i = RP * X_i \qquad \text{VI-3}$$

$$Var(X_i) = (CV_i * X_i)^2 \qquad \text{VI-4}$$

where

RP = relative perturbation for input variable X_i

CV = coefficient of variation for input variable X_i

X_i = value of input variable used in base case simulation

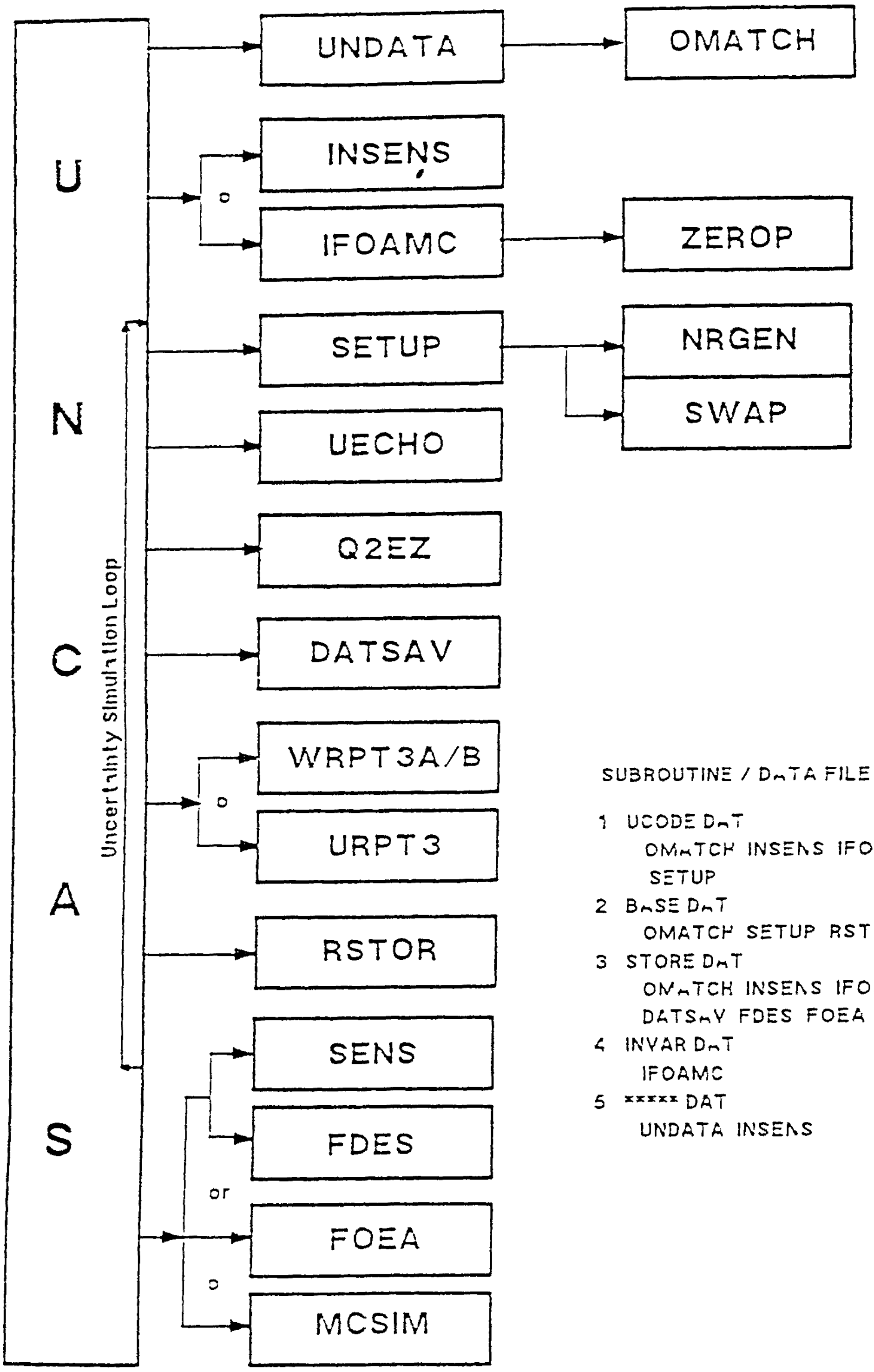
The specific manner in which the input data requirements are supplied to QUAL2E-UNCAS, including the data file "INVAR DAT," are described in Appendix B-User Manual for QUAL2E-UNCAS

6 1 PROGRAMMING STRATEGY IN QUAL2E-UNCAS

QUAL2E-UNCAS has been structured in a manner to minimize the tedious requirements for user adjustments to the QUAL2E input data file used in the base case simulation The UNCAS portion of QUAL2E-UNCAS consists of two parts (a) a package of 16 subroutines that perform the necessary book-keeping and computations as well as printing the uncertainty results and (b) one data file to decode and link UNCAS requests with QUAL2E The user must supply two input data files--the first provides the general specifications for the uncertainty analysis to be performed, and the second contains the input variance information In addition, during execution, UNCAS creates two disk files for storing and retrieving the simulation information used in computing the uncertainty analysis results The flow chart for UNCAS in Figure VI-1 shows the relationships among the subroutines and data files Each component of the UNCAS package and its function is described in the following sections

6 1 1 UNCAS Subroutines

a Subroutine UNCAS Subroutine UNCAS manages the execution of the uncertainty analysis simulations, computations, and output reports for QUAL2E-UNCAS It calls the appropriate subroutines for reading the uncertainty data files, for screening the input and output variables for consistency and compatibility with the QUAL2E model options selected in



SUBROUTINE / DATA FILE INTERACTIONS

1 UCODE DAT
OMATCH INSENS IFOAMC
SETUP
2 BASE DAT
OMATCH SETUP RSTOR SENS
3 STORE DAT
OMATCH INSENS IFOAMC
DATSAV FDES FOEA MCSIM
4 INVAR DAT
IFOAMC
5 ***** DAT
UNDATA INSENS

Figure VI-1 UNCAS Flow Diagram and Program Structure the base case simulation, for performing the uncertainty simulations, and for computing and printing the appropriate uncertainty results

b Subroutine UNDATA This subroutine reads the user-supplied input data file, ***** DAT, which contains the general specifications required for uncertainty analysis It sets the appropriate flags and conditions for the type of uncertainty analysis to be performed

c Subroutine OMATCH Subroutine OMATCH retrieves, purges, and stores (on disk file) the values of the appropriate output variables from the base case simulation For sensitivity analysis, it saves the complete output from the base case simulation in the file BASE DAT For first order error analysis and monte carlo simulation it stores only the values of the output variables at the locations (maximum of five) in the basin where uncertainty results are desired and only for those that were modeled in the base case simulation (STORE DAT) These data are subsequently used by subroutines DES, FOEA, and MCSIM for their respective uncertainty analysis computations

d Subroutine INSENS This subroutine controls the input specifications for sensitivity analysis It reads the user-supplied input data file, ***** DAT, for the input variables that are to be perturbed for sensitivity analysis It determines the total number of sensitivity simulations to be performed as well as the levels of all variables to be perturbed in each simulation

e Subroutine IFOAMC Subroutine IFOAMC controls the input specifications for first order error analysis and for monte carlo simulation It searches through a list of all input variables and purges (a) those variables that are not requested to be perturbed and (b) those input or model options that were not used in the base case simulation

f Subroutine ZEROP This subroutine examines the numerical value of each input variable If the value is such that the variable is not used in the base simulation (i e , zero, or 1 0 for a temperature coefficient), the input variable is purged from the uncertainty analysis simulations

g Subroutine SETUP Subroutine SETUP sets up the input condition for the current uncertainty simulation Using the list of relevant inputs developed in either INSENS or IFOAMC, each input variable is perturbed or randomized as specified It then calls subroutine SWAP to replace the base case value with the new value of the input variable

h Subroutine SWAP This subroutine swaps the newly perturbed or randomized value of the input variable(s) for the base value(s) Swapping is done in memory by input data type and EQUIVALENCED arrays Base case values are either saved in memory (sensitivity or first order options) or stored in the disk file BASE DAT (monte carlo)

i Subroutine NRGEN This subroutine generates either normally or log-normally distributed random numbers for each input variable to be randomized in a monte carlo simulation It uses a machine-specific random number generator i Subroutine UECHO Subroutine UECHO prints, as intermediate output, the input conditions of the current uncertainty simulation This output includes the name of the input variable being altered and its base and perturbed value This output is optional

k Subroutine Q2EZ This subroutine is not new to UNCAS It is that portion of the QUAL2E model that performs the simulation computations (see Figure I-1)

l Subroutine DATSAV This subroutine stores the appropriate output variables from each uncertainty simulation on the disk file STORE DAT, for later processing by FDES, FOEA, or MCSIM

m Subroutines WRPT3A and WRPT3B These subroutines are from the QUAL2E model, and write the final output summary for an UNCAS simulation This output is optional and is not available in the monte carlo option

n Subroutine URPT3 Subroutine URPT3 writes a limited intermediate output summary of each uncertainty simulation The summary consists of a comparison of (a) the steady state convergence characteristics for temperature and algae and (b) the base and new values of the output variables at the locations specified This output is optional and is available only for the sensitivity analysis using factorial design and first order error analysis

o Subroutine RSTOR This subroutine restores the value of the perturbed input to its base case value after completion of an uncertainty simulation Thus, it prepares the input data for the next UNCAS simulation

p Subroutine SENS Subroutine SENS writes the UNCAS final report for th sensitivity analysis option It is similar in format to the QUAL2E output pro duced by subroutines WRPT3A/B, but consists of the change in output variable (sensitivity) resulting from the input perturbations of the sensitivity analys

q Subroutine FDES This subroutine performs the analysis of a factorially designed set of sensitivity analysis simulations It writes the UNCAS final report for the factorial design, including the main and interaction effects of the sensitized input variables on each output variable at the user specified locations in the basin

r Subroutine FOEA Subroutine FOEA performs the computations and writes the UNCAS final report for the first order error analysis option The output consists of the normalized sensitivity coefficient matrix and the components of variance analysis for all inputs affecting each output variable at the user-specified locations in the basin

s Subroutine MCSIM This subroutine performs the computations and writes the UNCAS final report for the monte carlo simulation option The output consists of summary statistics, including base and simulated mean, bias, minimum, maximum, range, standard deviation, coefficient of variation, and skew coefficient as well as the frequency distribution (in one-half standard deviation steps) for each output variable at the user-specified locations in the basin

5 4 2 Internal UNCAS DATA Files

a File UCODE DAT This internal data file is supplied with the UNCAS package It is a master file that contains information for identifying, matching, and screening the inputs to be modified in an UNCAS simulation It also serves as the primary information source for linking UNCAS requests to the QUAL2E input data file

b File BASE DAT This internal data file stores information for the base case simulation In the sensitivity analysis option, it stores the values of all the output variables for the QUAL2E base simulation In the monte carlo simulation option, it stores the base values of the input variables that have been randomized This data file is not used with the first order error analysis option

c File STORE DAT This internal data file stores the values of output variables at the user-specified locations for the base simulation and for each uncertainty simulation When all uncertainty simulations are completed, these data are then used for the appropriate uncertainty output computations, i e , factorial design for the sensitivity analysis option, or normalized sensitivity coefficients and components of variance for the first order error analysis option, or summary statistics and frequency distributions for the monte carlo option

5 4 3 User-Supplied UNCAS Data Files

a File INVAR DAT This data file contains the uncertainty information for each input variable in QUAL2E These data consist of the variable name, its coefficient of variation, and its probability density function An example of this file, containing a set of default data, is provided with the UNCAS package Instructions for adjusting the uncertainty inputs to user specifications are provided in Appendix B--User Manual for QUAL2E-UNCAS

b File***** DAT This data file, named and prepared by the user, contains the general requirements for performing a QUAL2E-UNCAS simulation This information consists, in part, of specifying the uncertainty analysis option, the type of intermediate output, any constraints on input variables to be modified, the output variables and locations for computing and printing uncertainty results, the number of monte carlo simulations, and the magnitude of the input variable perturbation Instructions for assembling this data file are provided in Appendix B--User Manual for QUAL2E-UNCAS

5 5 LIMITATIONS AND CONSTRAINTS FOR QUAL2E-UNCAS

Because of the general purpose nature of the QUAL2E and UNCAS computer codes, there are a few constraints in using the models that arise from the program structure and bookkeeping strategies used These limitations are related to the level of detail the modeler may use in perturbing specific input variables

1 Reach or Source Variable Inputs and Forcing Functions In QUAL2E-UNCAS, input variables are treated in the general case rather than individually For example, if the user wishes to perform uncertainty analysis on the CBOD rate coefficient, or the point load flows, then all input values (over the entire basin) of the rate coefficient and flows are perturbed UNCAS does not have the capability of perturbing only one (or a few) of these inputs, i e , the value of the CBOD rate coefficient in reach 3 or the flows for the second and fourth point loads In short, the user specifies the name of the variable to be perturbed and the magnitude of the perturbation, then all values of that input variable are modified by the amount specified

2 First Order Error Analysis In first order error analysis, the user specifies the magnitude of the input perturbation, ΔX, for computing sensitivity coefficients UNCAS applies this value of ΔX uniformly to all input variables The modeler is not allowed to use one value of ΔX for one group of inputs and another value for a different group of inputs (Note The variance of each input variable can be specified uniquely, but as stated in subsection 1, that variance applies equally to all values of the variable in the basin)

3 Input Variables Having a Numerical Value of Zero Input variables whose values are determined by QUAL2E-UNCAS to be zero (either blanks in the input data file or an actual input value of zero) are assumed to be non-modeled inputs Those variables will not be perturbed in any UNCAS simulation, and thus will not contribute to the uncertainty of the modeled output

APPENDIX A

QUAL2E User Manual[*] [**]

The following sections illustrate the coding of input data forms for the QUAL2E model

A Title Data

All 16 cards are required in the order shown The first two are title cards and columns 22 through 80 may be used to describe the basin date of simulation etc Title cards 3 through 15 require either a YES" or NO" in columns 10 through 12 and are right justified Note that each of the nitrogen and phosphorus series must be simulated as a group

For each conservative substance (up to three) and the arbitrary non conservative the constituent name must be entered in columns 49 through 52 Corresponding input data units are entered in columns 57 through 60 (e g mg/L)

QUAL2E simulates ultimate BOD in the general case If the user wishes to use 5-day BOD for input and output the program will internally make the conversions to ultimate BOD This conversion is based upon first order kinetics and a decay rate that can be specified by the user (Type 1 Data Line 8) If no value is specified the program uses a default value of 0 23 per day base e It is recommended that users work only with ultimate BOD unless they have detailed knowledge of the river water and point source BOD kinetics To use the 5 day BOD input/output option write 5 DAY BIOCHEMICAL OXYGEN DEMAND" on the title 7 card beginning in column 22

Card 16 must read ENDTITLE beginning in column 1

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[*] From Modifications to the QUAL 2 Water Quality Model and User Manual for QUAL 2E Version 2 2 National Council of the Paper Industry for Air and Stream Improvement Inc New York NY NCASI Tech Bulletin No 457 April 1985 Used by permission

[**] Further modified to include enhancements to QUAL2E resulting in Version 3 0 of the model January 1987

B Data Type 1 Program Control

Type 1 Data define the program control options and the characteristics o the stream system configuration as well as some of the geographical/meteoro logical conditions for modeling temperature There are a maximum of 17 Data 1 cards The first 13 are required the last four are necessary only if temperature is being simulated

The QUAL2E program recognizes Type 1 Data by comparing the first four characters (columns 1-4) of each data card with a set of internally fixed codes If a match between the code and characters occurs then the data ar accepted as supplied on the card by the user If a match does not occur then the program control options will revert to default values and the system variables for the unmatched codes will be assigned a value of zero (0 0)

The first seven cards control program options If any characteristics <u>other</u> than those shown below are inserted in the columns 1 through 4 the actions described will <u>not</u> occur

LIST - Card 1 list the input data

WRIT Card 2 write the intermediate output report WRPT2 (see SUBROUTINE WRPT2 in the QUAL II documentation report (Roesner et al 1981) or NCASI Technical Bulletin No 391)

FLOW Card 3 use the flow augmentation option

STEA Card 4 shows this is a steady state simulation If it is <u>not</u> to be a steady-state write DYNAMIC SIMULATION or NO STEADY STATE and it is automatically a dynamic simulation

TRAP Card 5 cross sectional data will be specified for each reach If discharge coefficients are to be used for velocity and depth computa tions write DISCHARGE COEFFICIENTS or NO TRAPEZOIDAL CHANNELS beginning in column 1

PRIN Card 6 local climatological data specified for the basin simulation will appear in the final output listing

PLOT Card 7 dissolved oxygen and BOD will be plotted in final output listing

The next two cards provide further program flags and coefficients This information is supplied in two data fields per card columns 26 35 and 71 80 Note that the character codes in columns 1 4 must occur as shown in order for the data to be accepted by the program

FIXD Card 8 specifies (a) whether the downstream boundary water quality constituent concentrations are fixed (user specified), and (b) the value of the rate coefficient for converting input 5-day BOD to ultimate BOD. A value of 1.0 (or larger) in columns 26-35 specifies that the downstream boundary water quality constituent concentrations will be supplied in Data Types 13 and 13A. A value less than 1.0 (usually 0.0 or blank) in these columns means that the downstream boundary concentrations are not user specified. In this case, the concentrations in the most downstream element (Type 5) will be computed in the normal fashion using the zero gradient assumption (Section 5.4.3.2). The second value on this card, columns 71-80, is the rate coefficient for converting 5-day BOD to ultimate BOD. It is used only when 5-day BOD is being modeled (Title Card 7). If the columns are left blank, the model uses a default value of 0.23 per day, base e. Note that this conversion factor is applied to all input BOD_5 forcing functions (headwaters, incremental flows, point loads, and the downstream boundary condition).

INPU Card 9 specifies whether the input and/or output will be in metric or English units. The value of 1.0 (or larger) in card columns 26-35 specifies metric input. The value of 1.0 (or larger) in card column 71-80 specifies metric units for output. Any value less than 1.0 (usually 0.0 or blank) will specify English units.

The next four cards describe the stream system. There are two data fields per card, columns 26-35 and 71-80. The program restrictions on the maximum number of headwaters, junctions, point loads, and reaches are defined by PARAMETER statements in the Fortran code. These statements may be modified by the user to accommodate a particular computer system or QUAL2E simulation application. The values of the constraints in the code as distributed by EPA are:

Maximum number of headwaters	7
Maximum number of junctions	6
Maximum number of point loads	25
Maximum number of reaches	25
Maximum number of computational elements	250

NUMB Card 10 defines the number of reaches into which the stream is segmented and the number of stream junctions (confluences) within the system.

NUM_ Card 11 shows the number of headwater sources and the number of inputs or withdrawals within the system. The inputs can be small streams, wasteloads, etc. Withdrawals can be municipal water supplies, canals, etc. NOTE: Withdrawals must have a minus sign ahead of the flow in Data Type 11 and must be specified as withdrawals in Data Type 4 by setting IFLAG = 7 for that element. Note the code for Card 11 is NUM_ (read NUM space) to distinguish it from the code for Card 10, NUMB.

TIME Card 12 contains the time step interval in hours and the length of the computational element in miles (kilometers) The time step interval is used only for a dynamic simulation thus it may be omitte if the simulation is steady state

MAXI - Card 13 provides information with different meanings depending on whether a dynamic or a steady state simulation is being performed For a dynamic simulation the maximum route time is specified in columns 26 35 This value represents the approximate time in hours required for a particle of water to travel from the most upstream point in the system to the most downstream point The time increment in hours for intermediate summary reports of concentration profiles is specified in columns 71-80 For a steady-state simulation the maximum number of iterations allowed for solution convergence is entered in columns 26 35 The value in columns 71 80 may be left blank because it is not required in the steady-state solution

The next four cards provide geographical and meteorological informatio and are required only if temperature is being simulated There are two dat fields per card columns 26 35 and 71-80 Note the character codes in columns 1-4 must occur as shown in order for the data to be accepted by the program

LATI - Card 14 contains the basin latitude and longitude and represent mean values in degrees for the basin

STAN Card 15 shows the standard meridian in degrees and the day of the year the (Julian date) simulation is to begin

EVAP Card 16 specifies the evaporation coefficients Typical values are AE = 6 8 x 10^{-4} ft/hr in Hg and BE = 2 7 x 10^{-4} ft/hr in Hg-mph of wind for English units input or AE = 6 2 x10^{-6} m/hr-mbar and BE = 5 5 x 10^{-6} m/hr mbar m/sec of wind for metric units input

ELEV Card 17 contains the mean basin elevation in feet (meters) above mea sea level and the dust attenuation coefficient (unitless) for solar radiation The dust attenuation coefficient generally ranges between zero and 0 13 Users may want to consult with local meteorologists for more appropriate values

Note If the reach variable climatology option (steady state simulations only) is used the elevation data and dust attenuation coefficient for each reach are supplied in Data Type 5A and the value supplied in Data Type 1A are overridden

Data Type 1 must end with an ENDATA1 card

C Data Type 1A Global Algal, Nitrogen, Phosphorus, and Light Parameters

These parameters and constants apply to the entire simulation and represent the kinetics of the algal, nutrient, and light interactions. It is important to note that proper use of all options in QUAL2E requires detailed knowledge of the algal growth kinetics appropriate for the water body being simulated.

These data cards are required only if algae, the nitrogen series (organic, ammonia, nitrite, and nitrate), or the phosphorus series (organic and dissolved) are to be simulated. Otherwise they may be omitted except for the ENDATA1A card. Information is supplied in two data fields per card, columns 33-39 and 74-80. As with Type 1 Data, QUAL2E recognizes Type 1A Data by comparing the first characters (columns 1-4) of each card with a set of internally fixed codes. If a match between the codes and the characters occurs, then data are accepted as supplied on the card by the user. If a match does not occur, then the system variables for the unmatched codes will be assigned the value zero (0.0). Note: the spaces (under bars) are an integral (necessary) part of the four character code.

O_UP Card 1 specifies the oxygen uptake per unit of ammonia oxidation and oxygen uptake per unit of nitrite oxidation.

O_PR Card 2 contains data on oxygen production per unit of algae growth, usually 1.6 mg O/mg A, with a range of 1.4 to 1.8. It also contains data on oxygen uptake per unit of algae respiration, usually 2.0 mg O/mg A respired, with a range of 1.6 to 2.3.

N_CO Card 3 concerns the nitrogen content and phosphorus content of algae in mg N or P per mg of algae. The fraction of algae biomass that is nitrogen is about 0.08 to 0.09, and the fraction of algae biomass that is phosphorus is about 0.012 to 0.015.

ALG_ Card 4 specifies the growth and respiration rates of algae. The maximum specific growth rate has a range of 1.0 to 3.0 per day. The respiration value of 0.05 is for clean streams, while 0.2 is used where the N_T and P_2 concentrations are greater than twice the half saturation constants.

N_HA - Card 5 contains the nitrogen and phosphorus half saturation coefficients. The range of values for nitrogen is from 0.01 to 0.3 mg/L and for phosphorus the values typically range from 0.001 to 0.05 mg/L.

LIN_ Card 6 contains the linear and nonlinear algal selfshading light extinction coefficients. The coefficients λ_1 and λ_2 are defined below:

λ_1 - linear algae self shading coefficient
(1/ft)/(ug chla/L) or (1/m)/(ug chla/L)

λ_2 - nonlinear algae self shading coefficient
$(1/ft)/(ug\ chla/L)^{2/3}$ or $(1/m)/(ug\ chla/L)^{2/3}$

These two self-shading coefficients are used with λ_0 the non-algal light extinction coefficient (Type 6B Data) in the general light extinction equation shown below

$$\lambda = \lambda_0 + \lambda_1 \alpha_0 A + \lambda_2 (\alpha_0 A)^{2/3}$$

where λ is the total light extinction coefficient and A is the algae biomass concentration in mg A/L and α_0 is the chlorophyll a to algae biomass ratio as ug chla/mg A Appropriate selection of the values of λ_0 λ_1 and λ_2 allows a variety of light extinction relationships to be simulated as follows

- No self shading (Roesner et al SEMCOG)

  $\lambda_1 = \lambda_2 = 0$

- Linear algal self-shading (JRB Assoc Vermont)

  $\lambda_1 \neq 0 \quad \lambda_2 = 0$

- Nonlinear self-shading (Riley Eq metric units)

  $\lambda_1 = 0.0088$

  $\lambda_2 = 0.054$

LIGP Card 7 contains the solar light function option for computing the effects of light attenuation on the algal growth rate and the light saturation coefficient QUAL2E recognizes three different solar light function options The light saturation coefficient is coupled to the selection of a light function thus care must be exercised in specifying a consistent pair of values

The depth integrated form of the three light functions and the corresponding definitions of the light saturation coefficient are given in Section 3.2.3.1 Eq III-6a b c and outlined in the following table

Light Function Option (Columns 33 38)	Light Saturation Coefficient* (Columns 74-80)
1 (Half Saturation)	Half Saturation Coefficient
2 (Smith s Function)	Light intensity corresponding to 71% of maximum growth rate
3 (Steele s Function)	Saturation Light Intensity

* Units of the Light Saturation Coefficient are as follows
English BTU/ft^2 min and Metric Langleys/min

Light Function Option 1 uses a Michaelis Menton half saturation formulation for modeling the algal growth limiting effects of light (FL) It is the method used in the SEMCOG version of QUAL 2 Option 2 is similar to Michaelis Menton but uses a second order rather than first order light effect Both options 1 and 2 are monotonically increasing functions of light intensity Option 3 includes a photoinhibition effect at high light intensities and has been reported in Bowie et al (1985)

DAIL Card 8 contains the light averaging option (columns 33-39) and the light averaging factor (columns 74-80) These values are used only in a steady state simulation The light averaging option allows the user to specify the manner in which the light attenuation factor is computed from the available values of solar radiation (See Section 3 2 3 2) A summary of these options is given below

Option	Description
1	FL is computed from one daily average solar radiation value calculated in the steady state temperature subroutine (HEATER)
2	FL is computed from one daily average solar radiation read from Data Type 1A
3	FL is obtained by averaging the 24 hourly values of FL that are computed from the 24 hourly values of solar radiation calculated in the steady-state temperature subroutine (HEATER)
4	FL is obtained by averaging the 24 hourly values of FL that are computed from the 24 hourly values of solar radiation computed from the total daily solar radiation (Data Type 1A) and an assumed cosine function

Note that if options 1 or 3 are selected temperature must be simulated

The light averaging factor (columns 74 80) is used to make a single calculation using daylight average solar radiation (Option 1 or 2) agree with average of calculations using hourly solar radiation values (Option 3 or 4) The factor has been reported to vary from 0 85 to 1 00

The selection of a daily (diurnal) light averaging option depends largely on the detail to which the user wishes to account for the diurnal variation in light intensity Options 1 and 2 utilize a single calculation of FL based on an average daylight solar radiation value Options 3 and 4 calculate hourly values of FL from hourly values of solar radiation and then average the hourly FL values to obtain the average daylight value. Options 1 and 3 use the solar radiation from the temperature heat balance routines (thus both algae and temperature simulations draw on the same source for solar radiation). Options 2 and 4 use the solar radiation value in Data Type 1A for the algae simulation. Thus either option 2 or 4 must be selected when algae are simulated and temperature is not. The light averaging factor is used to provide similarity in FL calculations between options 1 and 2 versus options 3 and 4. The solar radiation factor (Data Type 1A, card 11) specifies the fraction of the solar radiation computed in the heat balance that is photosynthetically active. It is used only with options 1 or 3.

In dynamic algae simulations, option 3 is used (default) unless temperature is not simulated, in which case solar radiation data are read in with the local climatology data.

NUMB Card 9 contains the number of daylight hours (columns 33-39) and the total daily radiation (BTU/ft^2 or Langleys) (columns 74-80). This information is used if light averaging options 2 or 4 are specified for the simulation.

ALGY Card 10 contains the light-nutrient option for computing the algae growth rate (columns 33-39) and the algal preference factor for ammonia nitrogen (columns 74-80). The light-nutrient interactions for computing algae growth rate are as follows (see also Section 3.2.2):

Option	Description
1	Multiplicative: $(FL) \times (FN) \times (FP)$
2	Limiting Nutrient: $FL \times [\text{minimum} (FN, FP)]$
3	Harmonic Mean: $\dfrac{FL \times 2}{1/FN + 1/FP}$

Option 1 is the form used in QUAL-II SEMCOG, while option 2 is used in the revised META Systems Version of QUAL-II (JRB Associates, 1983). Option 3 is described by Scavia and Park (1976).

The algal preference factor for ammonia (columns 74-80) defines the relative preference of algae for ammonia and nitrate nitrogen (see also Section 3.3.2). The user defines this preference by specifying a decimal value between 0 and 1.0, for example:

Algal Preference Factor for Ammonia	Interpretation
0.0	Algae will use only nitrate for growth
0.5	Algae will have equal preference for ammonia and nitrate
1.0	Algae will use only ammonia for growth

ALG/ Card 11 contains the factor for converting the solar radiation value from the heat balance to the solar radiation value appropriate for the algae simulation (columns 33-39) and the value of the first order nitrification inhibition coefficient (columns 74 80)

The solar radiation factor specifies the fraction of the solar radiation computed in the heat balance (subroutine HEATER) that is photosynthetically active (i.e. used by algal cells for growth). It is required only in steady state simulations when light averaging options 1 or 3 (Data Type 1A card 8) are selected. A decimal value between 0 and 1.0 specifies the value of this fraction. Typically the value of this fraction is about 0.45 (Bannister 1974)

The first order nitrification inhibition coefficient is the value of KNITRF in the following equation (see Section 3.3.5)

$$CORDO = 1.0 - exp(-KNITRF * DO)$$

where

DO - dissolved oxygen concentration (mg/L) and
CORDO - correction factor applied to ammonia and nitrite oxidation rate coefficients

The following table contains values of CORDO as a function of DO (row) and KNITRF (column)

DO (mg/L)	KNITRF 0.5	0.7	1.0	2.0	5.0	10.0
0.1	.05	.07	.10	.18	.39	.63
0.2	.10	.13	.18	.33	.63	.86
0.3	.14	.19	.26	.45	.78	.95
0.4	.18	.24	.33	.55	.86	.98
0.5	.22	.30	.39	.63	.92	.99
0.7	.30	.39	.50	.75	.97	1.00
1.0	.39	.50	.63	.86	.99	1.00
1.5	.53	.65	.78	.95	1.00	1.00
2.0	.63	.75	.86	.98	1.00	1.00
3.0	.78	.88	.95	1.00	1.00	1.00
4.0	.86	.94	.98	1.00	1.00	1.00
5.0	.92	.97	.99	1.00	1.00	1.00
7.0	.97	.99	1.00	1.00	1.00	1.00
10.0	.99	1.00	1.00	1.00	1.00	1.00

A value of 0.6 for KNITRF closely matches the inhibition formulation in QUAL TX (TWDB 1984) while a value of 0.7 closely matches the data for the Thames Estuary (DSIR 1964). The default value of KNITRF is 10.0 i.e. no inhibition of nitrification at low dissolved oxygen

ENDA The last card in Data Type 1A must be an ENDATA1A card regardless of whether algae nitrogen or phosphorus are simulated

D Data Type 1B Temperature Correction Factors

Several of the processes represented in QUAL2E are affected by temperature The user may elect to input specific temperature correctio factors In the absence of such information default values are used as noted in Table A 1 The user need supply only those values that are to be changed

Data Type 1B information is supplied as follows

Alphanumeric code for each temperature coefficient as noted in Table A 1	Columns 10 17
User specified temperature coefficient	Columns 19 26

The last card in Data Type 1B must be an END-TA1B card regardless of whether any of the default values are modified

TABLE A 1 DEFAULT THETA VALUES FOR QUAL2E

INDEX	RATE COEFFICIENT	DEFAULT VALUES SIMCOG	 QUAL 2E	CODE
1	BOD Decay	1 047	1 047	BOD DECA
2	BOD Settling		1 024	BOD SETT
3	Reaeration	1 0159	1 024	OXY TRAN
4	SOD Uptake	-	1 060	SOD RATE
5	Organic N Decay		1 047	ORGN DEC
6	Organic N Settling		1 024	ORGN SET
7	Ammonia Decay	1 047	1 083	NH3 DECA
8	Ammonia Source		1 074	NH3 SRCE
9	Nitrite Decay	1 047	1 047	NO2 DECA
10	Organic P Decay		1 047	PORG DEC
11	Organic P Settling		1 024	PORG SET
12	Dissolved P Source		1 074	DISP SRC
13	Algae Growth	1 047	1 047	ALG GROW
14	Algae Respiration	1 047	1 047	ALG RESP
15	Algae Settling		1 024	ALG SETT
16	Coliform Decay	1 047	1 047	COLI DEC
17	Non cons Decay	1 047	1 000	ANC DECA
18	Non cons Settling		1 024	ANC SETT
19	Non cons Source	-	1 000	ANC SRCE

Data Type 2 - Reach Identification and River Mile/Kilometer Data

The cards of this group identify the stream reach system by name and river mile/kilometer by listing the stream reaches from the most upstream point in the system to the most downstream point. When a junction is reached, the order is continued from the upstream point of the tributary. There is one card per reach. The following information is on each card:

Reach Order or Number	Columns 16-20
Reach Identification or Name	Columns 26-40
River Mile/Kilometer at Head of Reach	Columns 51-60
River Mile/Kilometer at End of Reach	Columns 71-80

A very useful feature of QUAL2E pertaining to modifications of reach identification once the system has been coded is that existing reaches may be subdivided (or new reaches added) without renumbering the reaches for the whole system. If, for example, it is desired to divide the river reach originally designated as REACH 3 into two reaches, the division is made by calling the upstream portion REACH 3 and the new reach downstream REACH 3.1. Up to nine such divisions can be made per reach (3.1-3.9); thus REACH 3 (or any other reach) can be divided into as many as 10 reaches numbered 3, 3.1-3.9. This option of dividing a reach is useful particularly when new field data indicate a previously unknown change in geomorphology or when the addition of a new or proposed load alters the biochemistry in the downstream portion of the reach. If this option is invoked, the number of reaches specified in Data Type 1 must be changed to the new total number of reaches.

Note: It is important to realize that this option cannot be used to subdivide a reach into more (and thus smaller) computational elements in an attempt to provide greater detail to the simulation. All computational elements must have the same length (as specified in Type 1 Data).

This option also will allow the user to add a new reach to the system, for example, taking a tributary that was initially modeled as a point source and changing it to a modeled reach (or reaches) in the basin. This type of modification adds a junction to the system and thus the junction information in Data Types 1, 4, and 9 must be modified accordingly.

This group of cards must end with ENDATA2.

Data Type 3 - Flow Augmentation Data

These cards except ENDATA3 are required only if flow augmentation to be used The cards in this group contain data associated with determ flow augmentation requirements and available sources of flow augmentatio There must be as many cards in this group as in the reach identification group The following information is on each card

Reach Order or Number	Columns 26-30
Augmentation Sources (the number of headwater sources which are avail able for flow augmentation)	Columns 36-40
Target Level (minimum allowable dissolved oxygen concentration (mg/L) in this reach)	Columns 41-50
Order of Sources (order of avail- able headwaters starting at most upstream points	Columns 51-80

This card group must end with ENDATA3 even if no flow augmentation is desired

Data Type 4 Computational Elements Flag Field Data

This group of cards identifies each type of computational element in each reach These data allow the proper form of the routing equations to be used by the program There are seven element types allowed they are listed below

IFLAG	Type
1	Headwater source element
2	Standard element incremental inflow/outflow only
3	Element on mainstream immediately upstream of a junction
4	Junction element
5	Most downstream element
6	Input (point source) element
7	Withdrawal element

Each card in this group (one for each reach) contains the following information

Reach Order or Number	Columns 16-20
Number of Elements in the Reach	Columns 26-30
Element Type (these are the numbers (IFLAG above) which identify each element by type)	Columns 41-80

Remember that once a system has been coded reaches can be divided or new ones added without necessitating the renumbering of the entire system (see Data Type 2 - Reach Identification and River Mile/Kilometer Data for application and constraints) When this option is invoked the element types and number of elements per reach for the affected reaches must be adjusted in Data Type 4 to reflect the changes

This card group must end with ENDATA4

[illegible] Data Type 5 Hydraulics Data

Two options are available to describe the hydraulic characteristics of the system. The first option utilizes a functional representation whereas the second option utilizes a geometric representation. The option desired is specified in Data Type 1, card 5. The code "TRAPEZOIDAL" specifically denotes the geometric representation. Any other code, such as "NO TRAPEZOIDAL" or "DISCHARGE COEFFICIENTS", specifies the functional representation.

Note: With either option the effect is global (for the entire system). This option is not reach variable.

If the first option is selected, velocity is calculated as $V = aQ^b$ and depth is found by $D = cQ^d$. Each card represents one reach and contains the values of a, b, c and d as described below.

Reach Order or Number	Columns 16-20
Dispersion Constant	Columns 23-30
a coefficient for velocity	Columns 31-40
b exponent for velocity	Columns 41-50
c coefficient for depth	Columns 51-60
d exponent for depth	Columns 61-70
Manning's "n" for reach (if not specified, the program default value is 0.02)	Columns 71-80

The dispersion constant is the value of K in the general expression relating the longitudinal dispersion coefficient to the depth of flow and shear velocity (See Section 2.4.3).

$$D_L = Kdu^*$$

where

D_L = longitudinal dispersion coefficient (ft^2/sec, m^2/day)

K = dispersion constant, dimensionless

d = mean depth of flow (ft, m)

u^* = shear velocity (ft/sec, m/sec) = $(gdS)^{1/2}$

g = gravitational constant (ft/sec^2, m/sec^2)

S = slope of the energy grade line (ft/ft, m/m)

Substitution of the Manning equation for S leads to the following expression for the longitudinal dispersion coefficient D_L

$$D_L = 3\ 82\ Knud^{5/6}$$

where

n = Mannings roughness coefficient and

V = Mean stream velocity (ft/sec m/sec)

Typical values of K range from 6 to 6000 A value of 5 93 leads to the older equation for longitudinal dispersion which is the one used in the SEMCOG version of QUAL-II

The coefficients a b c and d should be expressed to relate velocity depth and discharge units as follows

System	Q	V	D
Metric	m^3/sec	m/sec	m
English	ft^3/sec	ft/sec	ft

If the second option is selected each reach is represented as a trapezoidal channel These data are also used to specify the trapezoidal cross-section (bottom width and side slope) the channel slope and the Manning's "n" corresponding to the reach The program computes the velocity and depth from these data using Manning's Equation and the Newton Raphson (iteration) method

One card must be prepared for each reach

Reach Order or Number	Columns 16-20
Dispersion Constant K	Columns 23-30
Side Slope 1 (run/rise ft/ft m/m)	Columns 31-40
Side Slope 2 (run/rise ft/ft m/m)	Columns 41 50
Bottom Width of Channel (feet meters)	Columns 51 60
Channel Slope (ft/ft m/m)	Columns 61 70
Mannings "n" (Default 0 020)	Columns 71 80

This group of data cards must end with an ENDATA5 card

4A Data Type 5A Temperature and Local Climatology Data

This group of data supplies the reach variable air temperature an climatological information for steady-state water temperature simulation If QUAL2E is to be used in the dynamic/diurnal mode the air temperature ai climatological inputs must be global constants and are supplied in a separ data file according to the format described in Section X Climatological Data The data in this group consist of geographical and meteorological da required for performing the energy balance for heat transfer across the ai water interface

There are three options in QUAL2E for providing the input variables fc steady state temperature simulation

Option 1 Reach Variable Temperature Inputs In this option the user specifies explicitly the values of the temperature simulation inputs for al reaches in the system One card (line of data) is necessary for each reach and contains the following information

Reach Order or Number	Columns 16-20
Reach Elevation (ft m)	Columns 25 31
Dust Attenuation Coefficient	Columns 32 38
Cloudiness fraction in tenths of cloud cover	Columns 39-45
Dry Bulb Air Temperature (° C)	Columns 46-52
Wet Bulb Temperature (° C)	Columns 53 59
Barometric (atmospheric) Pressure (inches hg millibars)	Columns 60-66
Wind Speed (ft/sec m/sec)	Columns 67 73

Option 2a Global Values Current Version of QUAL2E With this option the user may specify a single value for each of the temperature simulation inputs and QUAL2E will assume that these values apply to all reac in the system being modeled The required input data for this option is the same as that for option 1 with the exception that only one line of data is necessary

Option 2b Global Values Prior QUAL2E Versions The current version of QUAL2E will accept without modification input data files for steady-state temperature simulations from prior versions of QUAL2E Because prior versions treated the temperature simulation inputs as global constants so also will the current version In this option the required temperature simulation inputs are supplied according to the specifications in Section X Climatological Data

Option 3 Reach Variable Temperature Inputs with Estimation of Pressure Variation with Elevation In the case where reach variable temperature simulation inputs are desired but atmospheric pressure values are either unknown or unavailable QUAL2E has the capability of estimating the value of atmospheric pressure for each reach from its elevation and temperature These estimates are computed from the ideal gas law integrated at constant temperature and specific humidity over the change in elevation relative to a datum (see Section 4 8) The input requirements for this option are the same as for option 1 with the exception that the value of atmospheric pressure is supplied for only one reach This value serves as the datum or reference from which atmospheric pressures for the other reaches are estimated If this option is used the computed values of reach atmospheric pressure will appear in the QUAL2E echo-print of the input data

Notes

1 It is important to realize that the user does not explicitly specify whether options 1 2 or 3 for steady state reach variable temperature simulation are to be used Rather QUAL2E examines the format in which the temperature/climatology input information are provided in the input data file matches it with one of the options described above and then proceeds with the appropriate computational strategy

2 This data group (Data Type 5A) must end with ENDATA5A If option 2b is to be used (input data files from prior versions of QUAL2E) this data type is eliminated entirely Data Type 5A is also not allowed for dynamic/diurnal QUAL2E simulations

3 Values for elevation and dust attenuation coefficient appear in two places here in Data Type 5A and also in Data Type 1 The values in Data Type 5A are used with options 1 2a and 3 and always override those in Data Type 1 The values in Data Type 1 are used only in option 2b input data files from prior versions of QUAL2E

Type 6 BOD and DO Reaction Rate Constants Data

This group of cards includes reach information on the BOD decay rate coefficient and settling rate sediment oxygen demand as well as the meth of computing the reaeration coefficient Eight options for reaeration coefficient calculation are available (see Section 3 6 2) and are listed below

K2 OPT	Method
1	Read in values of K2
2	Churchill
3	O Connor and Dobbins
4	Owens Edwards and Gibbs
5	Thackston and Krenkel
6	Langbien and Durum
7	Use equation $K2 = aQ^b$
8	Tsivoglou Wallace

One card is necessary for each reach and contains the following information

Reach Order or Number	Columns 16 20
BOD Decay Rate Coefficient (1/day)	Columns 21 28
BOD Removal Rate by Settling (1/day)	Columns 29 36
Sediment Oxygen Demand (g/ft^2-day g/m^2 day)	Columns 37 44
Option for K2 (1 8 as above)	Columns 45 48
K2 (Option 1 only) Reaeration Coefficient per day base e 20C	Columns 49 56
a Coefficient for K2 (Option 7) or Coefficient for Tsivoglou (Option 8)	Columns 57 64
b Exponent for K2 (Option 7) or Slope of the Energy Gradient S_e (Option 8)	Columns 65 72

The units of a and b vary depending on whether option 7 or 8 is used and on whether the input data are in English or Metric units as follows

Units of a	English	Metric
Option 7 (Coefficient)	Consistent with flow in cfs	Consistent with flow in cms
Option 8 (Coefficient)	1/ft	1/m
Units of b	**English**	**Metric**
Option 7 (Exponent)	Consistent with flow in cfs	Consistent with flow in cms
Option 8 (S_e)	Dimensionless	Dimensionless

For option 8 (Tsivoglou's option) the energy gradient S_e need not be specified if a Manning "n" value was assigned under Hydraulic Data Type 5 S_e will be calculated from Manning s Equation using the wide channel approximation for hydraulic radius

This group of cards must end with ENDATA6

J Data Type 6 - N and P Coefficients

This group of cards is required if algae the nitrogen series (organi nitrogen ammonia nitrite and nitrate) or the phosphorus series (organic and dissolved) are to be simulated Otherwise they may be omitted Each card of this group one for each reach contains the follo information

Reach Order or Number	Columns 20-24
Rate Coefficient for Organic-N Hydrolysis (1/day)	Columns 25 31
Rate Coefficient for Organic-N Settling (1/day)	Columns 32 38
Rate Coefficient for Ammonia Oxidation (1/day)	Columns 39-45
Benthos Source Rate for Ammonia (mg/ft^2 day mg/m^2-day)	Columns 46 52
Rate Coefficient for Nitrite Oxidation (1/day)	Columns 53 59
Rate Coefficient for Organic Phosphorus Decay (1/day)	Columns 60 66
Rate Coefficient for Organic Phosphorus Settling (1/day)	Columns 67 73
Benthos Source Rate for Dissolved Phosphorus (as P mg/ft^2-day mg/m^2-day)	Columns 74-80

Note that the benthos source rates are expressed per unit of bottom area Other versions of QUAL-II use values per length of stream To conve to the areal rate divide the length value by the appropriate stream width

This group of cards must end with ENDATA6A even if algae nitrogen or phosphorus are not simulated

< Data Type 6B Algae/Other Coefficients

This group of cards is required if algae the nitrogen series the phosphorus series coliform or the arbitrary non conservative is to be simulated Otherwise they may be omitted Each card of the group one per reach contains the following information

Reach Order or Number	Columns 20-24
Chlorophyll a to Algae Ratio* (ug chla/mg algae)	Columns 25-31
Algal Settling Rate (ft/day m/day)	Columns 32-38
Non-Algal Light Extinction** Coefficient (1/ft 1/m)	Columns 39-45
Coliform Decay Coefficient (1/day)	Columns 46-52
Arbitrary Non-Conservative Decay Coefficient (1/day)	Columns 53 59
Arbitrary Non-Conservative Settling Coefficient (1/day)	Columns 60-66
Benthos Source Rate for Arbitrary Non-Conservative (mg/ft^2 day mg/m^2 day)	Columns 67-73

If not specified the QUAL2E default value is 50 ug Chl-a/mg algae

** If not specified the QUAL2E default value is 0 01 ft^{-1} which corresponds approximately to the extinction coefficient for distilled water

This group of cards must end with ENDATA6B even if algae nitrogen phosphorus coliform or the arbitrary non conservative are not simulated

Data Type 7 - Initial Conditions 1

This card group, one card per reach, establishes the initial conditions of the system with respect to temperature, dissolved oxygen concentration, BOD concentration and conservative minerals. Initial conditions for temperature must always be specified whether it is simulated or not. The reasons for this requirement are (a) when temperature is not simulated, the initial condition values are used to set the value of the temperature dependent rate constants, (b) for dynamic simulations, the initial conditions for temperature and every other quality constituent to be simulated define the state of the system at time zero, and (c) for steady state simulations of temperature, an initial estimate of the temperature between 35 F and 135 F is required to properly initiate the heat balance computations. Specifying 68F or 20C for all reaches is a sufficient initial condition for the steady state temperature simulation case. The information contained is as follows:

Reach Order or Number	Columns 20-24
Temperature (F or C)**	Columns 25-31
Dissolved Oxygen (mg/L)	Columns 32-38
BOD (mg/L)	Columns 39-45
Conservative Mineral I*	Columns 46-52
Conservative Mineral II*	Columns 53-59
Conservative Mineral III*	Columns 60-66
Arbitrary Non Conservative*	Columns 67-73
Coliform (No./100 ml)	Columns 74-80

* Units are those specified on the Title Card.

** If not specified, the QUAL2E default value is 68 F, 20 C.

This group of cards must end with ENDATA7.

Data Type 7A Initial Conditions 2

This group of cards is required if algae the nitrogen series or the phosphorus series are to be simulated The information is coded as follows

Reach Order or Number	Columns 20-24
Chlorophyll a (ug/L)	Columns 25-31
Organic Nitrogen as N (mg/L)	Columns 32-38
Ammonia as N (mg/L)	Columns 39 45
Nitrite as N (mg/L)	Columns 46-52
Nitrate as N (mg/L)	Columns 53-59
Organic Phosphorus as P (mg/L)	Columns 60-66
Dissolved Phosphorus as P (mg/L)	Columns 67 73

This group of cards must end with ENDATA7A even if algae nitrogen or phosphorus are not simulated

N. Data Type 8 Incremental Inflow 1

This group of cards one per reach accounts for the additional flows into the system not represented by point source inflows or headwaters These inflows which are assumed to be uniformly distributed over the reach are basically groundwater inflows and/or distributed surface runoff that ca be assumed to be approximately constant through time

An important new feature to QUAL2E is that incremental outflow along a reach may be modeled This option is useful when field data show a decreasing flow rate in the downstream direction indicating a surface flow contribution to groundwater

Each card one for each reach contains the following information

Reach Order or Number	Columns 20 24
Incremental Inflow (cfs m^3/sec) outflows are indicated with a minus sign	Columns 25 31
Temperature (° C)	Columns 32 38
Dissolved Oxygen (mg/L)	Columns 39-44
BOD (mg/L)	Columns 45 50
Conservative Mineral I	Columns 51 56
Conservative Mineral II	Columns 57 62
Conservative Mineral III	Columns 63 68
Arbitrary Non Conservative	Columns 69 74
Coliform (No /100 ml)	Columns 75 80

This group of cards must end with ENDATA8

Data Type 8A   Incremental Inflow - 2

This group of cards is a continuation of Data Type 8 and is required nly if algae the nitrogen series or the phosphorus series are to be mulated Each card one per reach contains the following information

Reach Order or Number	Columns 20-24
Chlorophyll a Concentration (ug/L)	Columns 25-31
Organic Nitrogen as N (mg/L)	Columns 32-38
Ammonia as N (mg/L)	Columns 39-45
Nitrite as N (mg/L)	Columns 46-52
Nitrate as N (mg/L)	Columns 53-59
Organic Phosphorus as P (mg/L)	Columns 60-66
Dissolved Phosphorus as P (mg/L)	Columns 67-73

This group of cards must end with ENDATA8A even if algae nitrogen or hosphorus are not simulated

P Data Type 9 Stream Junction Data

This group of cards is required if there are junctions or confluences i the stream being simulated Otherwise they may be omitted The junctions are ordered starting with the most upstream junction For systems containing a junction(s) on a tributary the junctions must be ordered the manner indicated in Figure A 1 that is the junctions must be ordered that the element numbers just downstream of the junction are specified in ascending order In Figure A-1 the downstream element numbers for Junctio 1 2 and 3 are 29 56 and 64 respectively There is one card per junctio and the following information is on each card

Junction Order or Number	Columns 21-25
Junction Names or Identification	Columns 35 50
Order Number of the Last Element in the reach immediately upstream of the junction (see Figure A 1) In the example for Junction 1 the order number of the last element immediately upstream of the junction is number 17 For Junction 2 it is number 49 For Junction 3 it is number 40	Columns 56-60
Order Number of the First Element in the reach immediately down stream from the junction It is these numbers that must be arranged in ascending order Thus for Figure A 1 these order numbers for Junctions 1 2 and 3 are 29 56 and 64 respectively	Columns 66 70
Order Number of the Last Element in the last reach of the tributary entering the junction For Figure A 1 these order numbers for Junctions 1 2 and 3 are 28 55 and 63 respectively	Columns 76 80

This group of cards must end with END-TP9 even if there are no junctions in the system

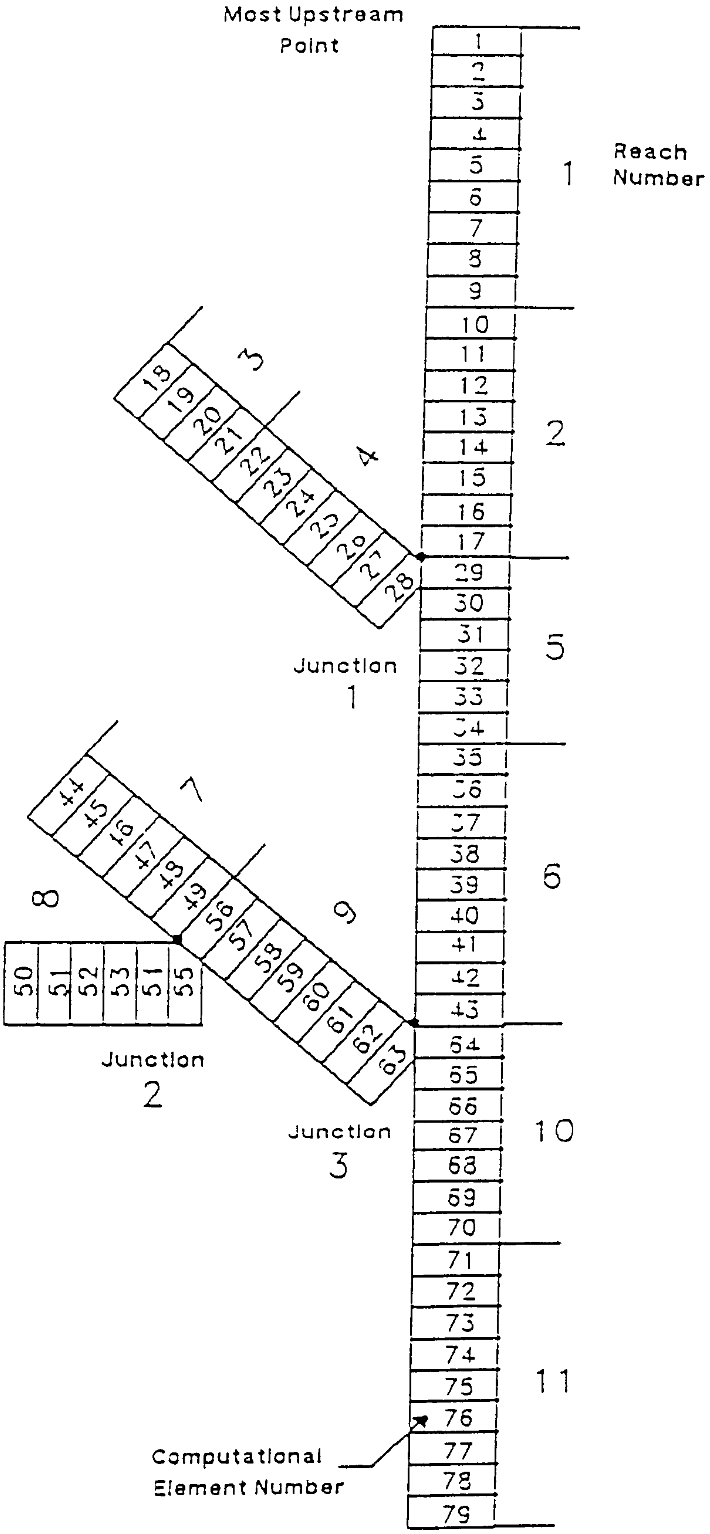


FIGURE A 1 STREAM NETWORK EXAMPLE TO ILLUSTRATE DATA INPUT

Q Data Type 10 Headwater Sources Data 1

This group of cards one per headwater defines the flow temperature dissolved oxygen BOD and conservative mineral concentrations of the headwater The following information is on each card

Headwater Order or Number Starting at Most Upstream Point	Columns 15 19
Headwater Name or Identification	Columns 20 35
Flow (cfs m^3/sec)	Columns 36-44
Temperature (F C)	Columns 45 50
Dissolved Oxygen Concentration (mg/L)	Columns 51-56
BOD Concentration (mg/L)	Columns 57 62
Conservative Mineral I	Columns 63-68
Conservative Mineral II	Columns 69-74
Conservative Mineral III	Columns 75-80

This group of cards must end with ENDATA10

R Data Type 10A Headwater Sources Data 2

This group of cards supplements the information in Data Type 10 and is required if algae the nitrogen series the phosphorus series, coliform or arbitrary non-conservative are to be simulated Each card one per headwater contains the following data

Headwater Order or Number	Columns 16-20
Arbitrary Non-Conservative	Columns 21-26
Coliform (No /100 ml)	Columns 27-32
Chlorophyll a (ug/L)	Columns 33-38
Organic Nitrogen as N (mg/L)	Columns 39-44
Ammonia as N (mg/L)	Columns 45-50
Nitrite as N (mg/L)	Columns 51-56
Nitrate as N (mg/L)	Columns 57 62
Organic Phosphorus as P (mg/L)	Columns 63-68
Dissolved Phosphorus as P (mg/L)	Columns 69-74

This group of cards must end with ENDATA10A even if algae nitrogen phosphorus coliform or arbitrary non-conservative are not simulated

S Data Type 11 Point Load)

This group of cards is used to define point source inputs and point withdrawals from the stream system Point sources include both wasteloads and unsimulated tributary inflows One card is required per inflow or withdrawal Each card describes the percent of treatment (for wastewater treatment) inflow or withdrawal temperature and dissolved oxygen BOD and conservative mineral concentrations They must be ordered starting at the most upstream point The following information is on each card

Point Load Order or Number	Columns 15-19
Point Load Identification or Name	Columns 20 31
Percent Treatment (applies only to influent BOD values)	Columns 32-36
Point Load Inflow or Withdrawal (cfs m^3/sec) (a withdrawal must have a minus ("-") sign	Columns 37-44
Temperature (° C)	Columns 45 50
Dissolved Oxygen Concentration (mg/L)	Columns 51 56
BOD Concentration (mg/L)	Columns 57-62
Conservative Mineral I	Columns 63-68
Conservative Mineral II	Columns 69 74
Conservative Mineral III	Columns 75-80

This group of cards must end with ENDATA11

Data Type 11A Point Load - 2

This group of cards supplements Data Type 11 and contains the algal nutrient coliform and arbitrary non-conservative concentrations of the point source loads This information is necessary only if algae the nitrogen series the phosphorus series coliform or the arbitrary non conservative are to be simulated Each card one per waste load (withdrawal) contains the following information

Point Load Order or Number	Columns 16-20
Arbitrary Non-Conservative	Columns 21-26
Coliform (No /100 ml)	Columns 27-32
Chlorophyll a (ug/L)	Columns 33-38
Organic Nitrate as N (mg/L)	Columns 39-44
Ammonia as N (mg/L)	Columns 45-50
Nitrite as N (mg/L)	Columns 51 56
Nitrate as N (mg/L)	Columns 57-62
Organic Phosphorus as P (mg/L)	Columns 63-68
Dissolved Phosphorus as P (mg/L)	Columns 69-74

This group of cards must end with ENDATA11A even if algae nitrogen phosphorus coliform or arbitrary non-conservative are not simulated

U Data Type 12 Dam Reaeration

This group of cards is required if oxygen input from reaeration over da is to be modeled as a component of the dissolved oxygen simulation Dam reaeration effects are estimated from the empirical equation attributed t Gameson as reported by Butts and Evans 1983 (see Section 3 6 5) The following inputs are required

Dam Order or Number	Columns 20-24
Reach Number of Dam	Columns 25 30
Element Number Below Dam	Columns 31-36
ADAM Coefficient ADAM - 1 80 for clean water - 1 60 for slightly polluted water - 1 00 for moderately polluted water - 0 65 for grossly polluted water	Columns 37-42
BDAM Coefficient BDAM - 0 70 to 0 90 for flat broad crested weir - 1 05 for sharp crested weir with straight slope face - 0 80 for sharp crested weir with vertical face - 0 05 for sluice gates with submerged discharge	Columns 43-48
Percent of Flow Over Dam (as a fraction 0 0 1 0)	Columns 49 54
Height of Dam (ft m)	Columns 55-60

This group of cards must end with ENDATA12 even if oxygen input from dam reaeration is not to be modeled

7 Data Type 13 Downstream Boundary 1

This data card supplies the constituent concentrations at the downstream boundary of the system It is required only if specified in Data Type 1 card 8 This feature of QUAL2E is useful in modeling systems with large dispersion in the lower reaches (e g estuaries) When downstream boundary concentrations are supplied the solution generated by QUAL2E will be constrained by this boundary condition If the concentrations are not provided the constituent concentrations in the most downstream element will be computed in the normal fashion using the zero gradient assumption (see Section 5 4 3 2)

Downstream boundary values for temperature dissolved oxygen BOD conservative mineral coliform and arbitrary non-conservative are required as follows

Temperature (° C)	Columns 25-31
Dissolved Oxygen (mg/L)	Columns 32 38
BOD Concentration (mg/L)	Columns 39-45
Conservative Mineral I	Columns 46-52
Conservative Mineral II	Columns 53-59
Conservative Mineral III	Columns 60-66
Arbitrary Non-Conservative	Columns 67-73
Coliform (No /100 ml)	Columns 74-80

This data group must end with an ENDATA13 card even if the fixed downstream boundary concentration option is not used in the simulation

Data Type 13A Downstream Boundary 2

This group of data (one card) is a continuation of Data Type 13 It required only if the fixed downstream boundary condition is used and if algae the nitrogen series and the phosphorus series are to be simulated This card contains the downstream boundary concentrations for algae nitrogen and phosphorus as follows

Chlorophyll *a* (ug/L)	Columns 25 31
Organic Nitrogen as N (mg/L)	Columns 32-38
Ammonia as N (mg/L)	Columns 39-45
Nitrite as N (mg/L)	Columns 46 52
Nitrate as N (mg/L)	Columns 53 59
Organic Phosphorus as P (mg/L)	Columns 60-66
Dissolved Phosphorus as P (mg/L)	Columns 67 73

This data group must end with an ENDATA13A card even if the fixed downstream boundary condition is not used and if algae nitrogen or phosphorus are not simulated

Climatological Data

Climatological data are required for

1 Temperature simulations, both steady-state and dynamic
2 Dynamic simulations where algae is being simulated and temperature is not

If neither temperature nor dynamic algae are being simulated, these cards may be omitted

For steady state temperature simulations these data may be supplied here (as in prior versions of QUAL2E) or in Data Type 5A but not both If the data are provided at this point in the input file QUAL2E assumes that the climatological inputs are global constants Only one card (line of data) is required which gives the basin average values of climatological data as follows

Month	Columns 18-19
Day	Columns 21 22
Year (last two digits)	Columns 24-25
Hour of Day	Columns 26-30
Net Solar Radiation* (BTU/ft^2 or Langleys/hour)	Columns 31 40
Cloudiness** fraction in tenths of cloud cover	Columns 41 48
Dry Bulb Temperature** (F C)	Columns 49-56
Wet Bulb Temperature** (F C)	Columns 57 64
Barometric pressure** (inches Hg millibars)	Columns 65-72
Wind speed** (ft/sec m/sec)	Columns 73-80

* Required only if dynamic algae is simulated and temperature is not

** Required if temperature is simulated

For dynamic/diurnal simulations the climatological input data must be read from a separate input file (FORTRAN Unit Number 2) This input procedure is different from that used with prior versions of QUAL-II and QUAL2E and is designed to assist user interaction with QUAL2E by modularizing the variety of input data QUAL2E may require The time variable climatology input data file is structured in the following manner The first line consists of a descriptive title (80 alphanumeric characters) that identifies the data contained in the file Subsequent lines provide the time variable basin average climatology data chronologically ordered at 3-hour intervals There must be a sufficient number of lines of data to cover the time period specified for the simulation (Data Type 1 card 13 MAXIMUM ROUTE TIME) The format for these data is the same as that described above for steady state temperature simulations

There is no ENDATA line required for the climatological data

Plot Reach Data

This data type is required if the plotting option for DO/BOD is selected (Data Type 1 card 7 PLOT DO/BOD) The following information is required for QUAL2E to produce a line printer plot

1 Card 1 BEGIN RCH
   Reach number at which plot is to begin — Columns 11-15

2 Card 2 PLOT RCH

   a Reach numbers in their input order (1 2 3 NREACH) — Columns 11-15, Columns 16-20, 21-26, etc, 76 80

   b If a reach is not to be plotted (i e a tributary) replace the reach number with a zero

   c Use additional PLOT RCH cards if there are more than 14 reaches in the system

3 Additional plots can be obtained by repeating the sequence of BEGIN RCH and PLOT RCH cards

As an example of the plotting option suppose that for the river system shown in Figure A 1 one wishes to obtain two DO/BOD plots one for the main stream (Reaches 1 2 5 6 10 and 11) and one for the second tributary (Reaches 7 and 9) The plot data would appear in the following order

```
BEGIN RCH 1
PLOT RCH 1  2  0  0  5  6  0  0  0  10  11
BEGIN RCH 7
PLOT RCH 0  0  0  0  0  0  7  0  9  0  0
```

No ENDATA card is required for the PLOT information

Y4 Plot Observed Dissolved Oxygen Data. The current version of QUAL2E has the capability to plot observed values of dissolved oxygen concentrations on the line printer plots produced for the computed values from the model. This feature is useful in assisting the user in model calibration. The observed DO data are read from a separate input data file (FORTRAN unit number 2) structured in a manner to be compatible with the Plot Reach Data (Section Y).

The first line, "DO TITLE," consists of a descriptive title (70 alphanumeric characters) that identifies the data contained in the file. The second line, "NUM LOCS," specifies the number of locations (n_1) for the first plot for which observed DO data are available. The next n_1 lines, "DO DATA," provide the observed DO data plotting information. One line is required for each location and contains the following data:

River location (mi, km)	Columns 11-20
Minimum DO (mg/L)	Columns 21-30
Average DO (mg/L)	Columns 31-40
Maximum DO (mg/L)	Columns 41-50

If only a single value of DO is available at a given location, it may be entered in either the minimum or average data position. Then by default QUAL2E will set the minimum, maximum, and average values all equal to the value entered. When more than one line printer plot is specified in the Plot Reach Data, the observed DO values for these plots are provided on the lines following that for the first plot. The information is entered by repeating the sequence of "NUM LOCS" and "DO DATA" lines for the data in the current plot.

Z Summary

Constructing a consistent and correct input data set for a QUAL2E simulation must be done with care This user's guide is designed to assist the user in this process It has been NCASI's and EPA's experience that two of the most frequently made errors in constructing a QUAL2E input data set are

(a) Using a numerical value that is inconsistent with the input units option selected, and

(b) Not adhering to the 4 character input codes for Data Types 1 and 1A

As an aid to the units problem Table A-2 is included in this report It provides a complete summary of all the input variables whose dimensions are dependent on whether English or metric units are selected Finally the user is encouraged to check and recheck the input codes in Data Types 1 and 1A for accuracy especially the codes for cards 10 and 11 of Data Type 1 (i e NUMB' and NUM_)

TABLE A 2 LIST OF QUAL2 INPUT VARIABLES THAT ARE ENGLISH/METRIC UNIT DEPENDENT

Data Type	Card or Line	Variable Description	FORTRAN Code Name	Units English	Units Metric
1	8	Input Units Specification	METRIC	0	1
	8	Output Units Specification	METOUT	0	1
1	11	Length of Computational Element	DELX	mile	kilometer
1	15	Evaporation Coefficient	AE	ft/hr in Hg	m/hr mbar
	15	Evaporation Coefficient	BE	ft/hr in Hg mph	m/hr mbar m/sec
1	16	Basin Elevation	ELEV	ft	meters
1A	6	Linear Algal Extinction Coeff	EXALG1	1/ft ug Chla/L	1/m ug Chla/
	6	Non linear Algal Extinction Coefficient	EXALG2	1/ft (ug Chla/L)$^{2/3}$	1/m (ug Chla/
1A	7	Light Saturation Coefficient	CKL	BTU/ft^2 min	langley/mi
1A	9	Total Daily Solar Radiation	SONET	Btu/ft^2	langleys
2	all	River Mile/km to Head of Reach	RMTHDR	mile	kilometer
	all	River Mile/km to End of Reach	RMTEDR	mile	kilometer
5 (Discharge Coefficient)	all	Coefficient on Flow for Velocity Exponent on Flow for Velocity Coefficient on Flow for Depth Exponent on Flow for Depth	COEFQV EXPOQV COEFQH EXPOQH	Consistent with flow velocity and depth in cfs fps ft respectively	Consistent with flow velocity and depth in cms mps m respectively
5 (Trapezoidal)	all	Bottom Width of Channel	WIDTH	ft	meters
5A	all	Reach Elevation	RCHELV	ft	meters
		Dry Bulb Temperature	RCHTDB	F	C
		Wet Bulb Temperature	RCHTWB	F	C
		Barometric Pressure	RCHATM	in Hg	mbar
		Wind Speed	RCHWND	ft/sec	m/sec
6	all	SOD Rate	CK4	gm/ft^2 day	gm/m^2 day
6	all	Option 7 for k_2 Coefficient on flow for k_2 Exponent on flow for k_2	COEQK2 EXPQK2	Consistent with flow in cfs	Consistent with flow in cms
6	all	Option 8 for K_2 Coefficient for Tsivoglou Eq Slope of Energy Gradient	COEQK2 EXPQK2	1/ft ft/ft	1/meter meter/meter
6A	all	Benthal Source Rate for Ammonia N	SNH3	mg/ft^2 day	mg/m^2 day
		Benthal Source Rate for Phosphorus	SPHOS	mg/ft^2 day	mg/m^2 day
6B	all	Algal Settling Rate	ALGSET	ft/day	m/day
		Non algal Extinction Coefficient	EXCOEF	1/ft	1/meter
		Arbitrary Nonconservative Benthal Source Rate	SRCANC	mg/ft^2 day	mg/m^2 day
7	all	Initial Condition Temperature	TINIT	F	C
8	all	Incremental Inflow			
		Flow Rate	QI	cfs	cms
		Temperature	TI	F	C
10	all	Headwater Conditions			
		Flow Rate	HWFLOW	cfs	cms
		Temperature	HWTEMP	F	C
11	all	Point Source/Withdrawal			
		Flow Rate	WSFLOW	cfs	cms
		Temperature	WSTEMP	F	C
2	all	Height of Dam	HDAM	ft	meters
13	1	Downstream Boundary Temperature	LBTEMP	F	C
LCD	all	Solar Radiation	SOLHR	Btu/ft^2 hr	langleys/hr
		Dry Bulb Temperature	DRYBLB	F	C
		Wet Bulb Temperature	WETBLB	F	C
		Barometric Pressure	ATMPR	in Hg	mbar
		Wind Speed	WIND	ft/sec	m/sec

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ① of ④

TITLE DATA

CARD TYPE	SIMULATE YES/NO	ALPHANUMERIC NAME	PARAMETER NAME	UNITS
TITLE01		TITLE OF RUN		
TITLE02		NAME OF BASIN		
TITLE03		CONSERVATIVE MINERAL I		
TITLE04		CONSERVATIVE MINERAL II		
TITLE05		CONSERVATIVE MINERAL III		
TITLE06		TEMPERATURE		
TITLE07		BIOCHEMICAL OXYGEN DEMAND		
TITLE08		ALGAE AS CHL-A IN UG/L		
TITLE09		PHOSPHORUS CYCLE AS P IN MG/L		
TITLE10		(ORGANIC-P, DISSOLVED-P)		
TITLE11		NITROGEN CYCLE AS N IN MG/L		
TITLE12		(ORGANIC-N, AMMONIA-N, NITRITE-N, NITRITE-N)		
TITLE13		DISSOLVED OXYGEN IN MG/L		
TITLE14		FECAL COLIFORMS IN NO./100 ML		
TITLE15		ARBITRARY NON-CONSERVATIVE		
ENDTITLE				

FORMAT (20A4)

NOTE The nitrogen cycle variables and the phosphorus cycle variables must each be simulated as a group

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ② of ㉔

DATA TYPE 1 PROGRAM CONTROL DATA

PROGRAM CONTROL PARAMETER	VALUE		PROGRAM CONTROL PARAMETER	VALUE
LIST DATA INPUT			[illegible]	
WRITE OPTIONAL SUMMARY			[illegible]	
NO FLOW AUGMENTATION			[illegible]	
STEADY STATE			[illegible]	
[illegible]			[illegible]	

FORMAT (6A4 A1 F10 0 10X 6A4 A1 F10 0)

X These lines may be omitted if temperature is not simulated

PARAMETER	ENGLISH UNITS	METRIC UNITS
Length of Computational Element	miles	kilometers
Evaporation Coef AE	(ft/hr)/(in Hg)	(m/hr)/(millibar)
Evaporation Coef BE	(ft/hr)/(in Hg mi/hr)	(m/hr)/(mbar m/sec)
Elevation of Basin	feet	meters

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ③ of ㉔

DATA TYPE 1A GLOBAL A N AND P PARAMETERS*

PARAMETER	VALUE	PARAMETER	VALUE
O UPTAKE BY NH3 OXID (MG O/MG N)		O UPTAKE BY NO2 OXID (MG O/MG N)	
O PROD BY ALGAE (MG O/MG A)		O UPTAKE BY ALGAE (MG O/MG A)	
N CONTENT OF ALGAE (MG N/MG A)		P CONTENT OF ALGAE (MG P/MG A)	
ALG MAX SPEC GROWTH RATE (1/DAY)		ALGAE RESPIRATION RATE (1/DAY)	
N HALF SATURATION CONST (MG/L)		P HALF SATURATION CONST (MG/L)	
LIN ALG SHADE CO (1/H-UGCHA/L)		NLIN SHADE (1/H-(UGCHA/L)**2/3)	
LIGHT FUNCTION OPTION (LFNOPT)		LIGHT SATURATION COEF (INT/MIN)	
DAILY AVERAGING OPTION (LAVOPT)		LIGHT AVERAGING FACTOR (INT)	
NUMBER OF DAYLIGHT HOURS (DLH)		TOTAL DAILY SOLAR RADTN (INT)	
ALGY GROWTH CALC OPTN (LGROPT)		ALGAL PREF FOR NH3-N (PREFN)	
ALG/TEMP SOLR RAD FACTOR (TFACT)		NITRIFICATION INHIBITION COEF	
ENDATA1A			

FORMAT (8A4 F7.0 2X 8A4 F7.0)

*Data Type 1A information except the ENDATA1A may be omitted unless algae nitrogen or phosphorus are to be simulated

Units Notation H depth, INT = light intensity

PARAMETER	ENGLISH UNITS	METRIC UNITS
Linear Algae Self Shade Coef	1/ft ugChla/l	1/m ugChla/l
Nonlinear Algae Self Shade Coef	$1/ft\ (ugChla/l)^{2/3}$	1/m (ugChla/l)
Light Saturation Coefficient (PAR)	Btu/ft^2 min	Langleys/min
Total Daily Solar Radiation (PAR)	Btu/ft^2	Langleys

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ① of ㉑

DATA TYPE 1B THETA VALUES

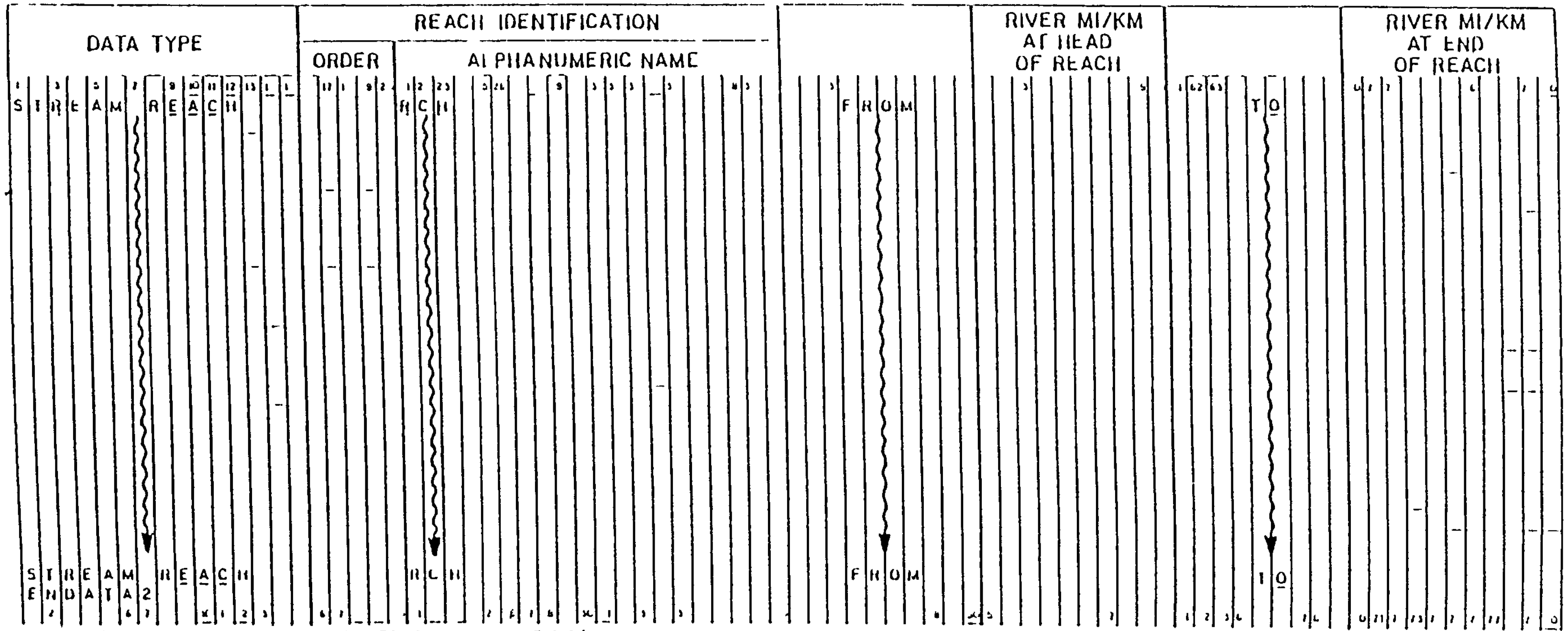
DATA TYPE	CODE	VALUE
THETA		
THETA		
ENDATA1B		

FORMAT (2A4 1X 2A4 1X F8.0)

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ⑤ of ㉔

DATA TYPE 2 REACH IDENTIFICATION DATA



FORMAT (3A4 3X F5.0 5A4 3X A4 3X F10.0 4X A2 4X F10.0)

NOTE Once data has been coded reaches may be subdivided without having to renumber the whole system see text for intructions

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM (F) of (24)

DATA TYPE 3 FLOW AUGMENTATION DATA

DATA TYPE	ORDER OF REACH		NO OF AUGMENT SOURCES AVAIL	TARGET LEVEL DISSOLVED OXYGEN (MG/L)	ORDER OF AVAILABLE AUGMENTATION SOURCES					
					1st	2nd	3rd	4th	5th	6th
FLOW AUGMT SOURCES RCH										
FLOW AUGMT SOURCES RCH										
ENDATA3										

FORMAT (5A4 5X F5.0 5X F5.0 F10.0 6F5.0)

These cards (except ENDATA3) may be deleted if flow augmentation is not used

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ⑦ of ㉔

DATA TYPE 4 COMPUTATIONAL ELEMENT FLAG FIELD DATA

DATA TYPE	ORDER OF REACH	'	NO OF COMP ELEM		COMPUTATIONAL ELEMENT FLAGS 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
FLAG FIELD RCH					
FLAG FIELD RCH					
ENDATA4					

FORMAT (2A4 A2 5X F5.0 5X F5.0 10X 20F2.0)

NOTE If subdivision of reaches is necessary after initial system has been coded it can be done without renumbering the entire system see text under REACH INDENTIFICATION AND RIVER MI/KM DATA

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ⑧ of ㉔

DATA TYPE 5 HYDRAULIC DATA

TRAPAZOIDAL CHANNELS	ORDER OF REACH		DISPN CONST	SIDE SLOPE 1	SIDE SLOPE 2	WIDTH (FEET, METERS)	SLOPE	MANNINGS N
DISCHARGE COEFFICIENTS	ORDER OF REACH		DISPN CONST	COEF ON Q FOR VELOCITY	EXPO ON Q FOR VELOCITY	COEF ON Q FOR DEPTH	EXPO ON Q FOR DEPTH	MANNINGS N
HYDRAULICS RCH								
HYDRAULICS RCH								
ENDATA5								

FORMAT (2A4 A2 5X F5 0 2X F8 0 5F10 0)

NOTE The discharge coefficients must be expressed to relate flow velocity and depth units as follows

VARIABLE	ENGLISH UNITS	METRIC UNITS
Flow	ft^3/sec	m^3/sec
Velocity	ft/sec	m/sec
Depth	ft	m

EPA/NCASI STREAM QUALITY ROUTING MODEL   QUAL2E INPUT DATA CODING FORMS

FORM (8a) of (24)

DATA TYPE 5A TEMPERATURE AND LOCAL CLIMATOLOGY DATA

DATA TYPE	ORDER OF REACH		ELEVATION	DUST ATTN COEF	CLOUDINESS	DRY BULB TEMP	WET BULB TEMP	BAROMETRIC PRESSURE	WIND SPEED	(not used)
TEMP/LCD RCH										
TEMP/LCD RCH										
ENDATA5A										

FORMAT (2A4 A2 5X F5.0 4X 8F7.0)

VARIABLE	ENGLISH UNITS	METRIC UNITS
Elevation	ft	m
Drybulb Wetbulb Temps	F	C
Barometric Pressure	in Hg	millibars
Wind Speed	ft/sec	m/sec

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ⑨ of ㉑

DATA TYPE 6 BOD/DO COEFFICIENTS

DATA TYPE	ORDER OF REACH	BOD DECAY COEF (1/DAY)	BOD SETT COEF (1/DAY)	SOD* RATE	K2 OPT	REAERATION COEF (1/DAY)	*COEQK2 or TSIV COEF FOR OPT 8	*EXPQK2 or SLOPE FOR OPT 8	(not used)
REACT COEF RCH									
REACT COEF RCH									
ENDATA6									

FORMAT (2A4 A2 5X F5.0 3F8.0 F4.0 3F8.0)

VARIABLE *	ENGLISH UNITS	METRIC UNITS
SOD Rate	gm/ft² day	g/m² day
COEQK2, EXPQK2 (Opt 7)	consistent with flow in ft³/sec	consistent with flow in m³/sec
TSIVC COEF (Opt 8)	1/ft	1/m
SLOPE (Opt 8)	ft/ft	m/m

EPA/NCASI STREAM QUALITY ROUTING MODEL — QUAL2E INPUT DATA CODING FORMS

FORM ⑩ of ㉔

DATA TYPE 6A N AND P COEFFICIENTS

DATA TYPE	ORDER OF REACH	ORG N HYDROLYSIS (1/DAY)	ORG N SETT COEF (1/DAY)	NH 3 OXIDATION (1/DAY)	BENTHAL SOURCE NH 3 *	NO 2 OXIDATION (1/DAY)	ORG P DECAY (1/DAY)	ORG P SETT COEF (1/DAY)	BENTHAL SOURCE DIS P *
N AND P COEF RCH									
END DATA 6A									

FORMAT (3A4 A2 5X F5 0 8F7 0)

VARIABLE *	ENGLISH UNITS	METRIC UNITS
Benthal Source for NH3 N	mg/ft² day	mg/m² day
Benthal Source for DIS P	mg/ft² day	mg/m² day

EPA/NCASI STREAM QUALITY ROUTING MODEL — QUAL2E INPUT DATA CODING FORMS

FORM (11) of (24)

DATA TYPE 6B ALGAE/OTHER COEFFICIENTS

DATA TYPE	ORDER OF REACH	CHLA TO ALGAE RATIO	*ALGY SETT RATE	*NON ALGAL LIGHT EXT COEF	COLI DECAY (1/DAY)	ANC DECAY (1/DAY)	ANC-SETT COEF (1/DAY)	* BENTHAL SOURCE ANC	(not used)
ALG/OTHER COEF RCH									
ALG/OTHER COEF RCH									
ENDATA6B									

FORMAT(3A4 A2 5X F5 0 7F7 0)

* VARIABLE	ENGLISH UNITS	METRIC UNITS
Algal Settling Rate	ft/day	m/day
Non algal Light Extinction Coef	1/ft	1/m
Benthal Source for Arbitrary Non Cons	mg Anc/ft² day	mg Anc/ft² day

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM (12) of (24)

DATA TYPE 7 INITIAL CONDITIONS-1

DATA TYPE	ORDER OF REACH	TEMP (F, C)	DISOLVED OXYGEN (MG/L)	BOD (MG/L)	CONS 1	CONS 2	CONS 3	ANC	COLIFORM (NO / 100 ML)
INITIAL COND RCH									
INITIAL COND RCH									
ENDATA7									

FORMAT(3A4 A2,5X,F5 0 8F7 0)

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ⑬ of ㉔

DATA TYPE 7A INITIAL CONDITIONS-2

DATA TYPE	ORDER OF REACH	CHL A (μG/L)	ORG N (MG/L)	NH_3-N (MG/L)	NO_2-N (MG/L)	NO_3-N (MG/L)	ORG P (MG/L)	DIS P (MG/L)	(not used)
INITIAL COND-2 RCH									
INITIAL COND-2 RCH									
ENDATA7A									

FORMAT (3A4 A2 5X F5.0 7F7.0)

EPA/NCASI STREAM QUALITY ROUTING MODEL — QUAL2E INPUT DATA CODING FORMS

FORM ⑭ of ㉔

DATA TYPE 8 INCREMENTAL FLOW 1

DATA TYPE	ORDER OF REACH	*INCREM FLOW	*TEMP	DISSOLVED OXYGEN (MG/L)	BOD (MG/L)	CONS 1	CONS 2	CONS 3	ANC	COLIFORM (NO / 100ML)
INCR INFLOW RCH										
INCR INFLOW I RCH										
ENDATA8										

FORMAT (3A4 A2 5X F5 0 2F7 0 7F6 0)

*VARIABLE	ENGLISH UNITS	METRIC UNITS
Incremental Flow	ft³/sec	m³/sec
Temperature	F	C

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ⑬ of ㉔

DATA TYPE 8A INCREMENTAL FLOW 2

DATA TYPE	ORDER OF REACH	CHL-A (μG/L)	ORG N (MG/L)	NH3-N (MG/L)	NO2-N (MG/L)	NO3 N (MG/L)	ORG P (MG/L)	DIS P (MG/L)	(not used)
INCR INFLOW-2 RCH									
INCR INFLOW 2 RCH									
ENDATA8A									

FORMAT (3A4 A2 5X F5.0 7F7.0)

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

DATA TYPE 9 STREAM JUNCTION DATA

FORM ⑯ of ㉔

DATA TYPE	ORDER OF JUNCTION		JUNCTION IDENTIFICATION		ELEMENT TYPE TYPE 3 NO OF ELEMENT UPSTRM OF JUNC		TYPE 4 NO OF ELEMENT DNSTRM OF JUNC		TYPE 2 NO OF ELEMENT ON TRIB
STREAM JUNCTION			JNC						
STREAM JUNCTION ENDATA9			JNC						

FORMAT (3A4 A3 5X F5 0 5X 5A4 3(5X F5 0)

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ⑰ of ㉔

DATA TYPE 10 HEADWATER-1

DATA TYPE	ORDER OF HDW	ALPHANUMERIC NAME	HEADWATER FLOW*	TEMP*	DISSOLVED OXYGEN (MG/L)	BOD (MG/L)	CONS1	CONS2	CONS3
HEADWTR 1 HDW									
HEADWTR HDW									
ENDATA10									

FORMAT (2A4 A2 4X F5.0 4A4 F9.0 6F6.0)

*VARIABLE	ENGLISH UNITS	METRIC UNITS
Headwater Flow	ft³/sec	m³/sec
Temperature	F	C

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM (18) of (24)

DATA TYPE 10A HEADWATER-2

DATA TYPE	ORDER OF HDW	ANC	COLI (NO / 100 ML)	CHL A (µG/L)	ORG N (MG/L)	NH3 N (MG/L)	NO2 N (MG/L)	NO3 N (MG/L)	ORG P (MG/L)	DIS P (MG/L)	(not used)
HEADWTR 2 HDW											
HEADWTR 2 HDW											
ENDATA10A											

FORMAT (2A4 A2 5X F5.0 9F6.0)

EPA/NCASI STREAM QUALITY ROUTING MODEL — QUAL2E INPUT DATA CODING FORMS

FORM ⑲ of ㉔

DATA TYPE 11 POINT LOAD AND WITHDRAWAL-1

DATA TYPE	ORDER OF LOAD	ALPHANUMERIC NAME	% TREATMENT	INFLOW or WITHDRAWAL *	TEMP *	DISSOLVED OXYGEN (MG/L)	BOD (MG/L)	CONS 1	CONS 2	CONS 3
P O I N T L D I I T L										
E N D A T A I i										

FORMAT (2A4 A1 5X F5 0, 3A4 F5 0 F8 0 6F6 0)

* VARIABLE	ENGLISH UNITS	METRIC UNITS
Inflow or withdrawal	ft^3/sec	m^3/sec
Temperature	F	C

EPA/NCASI STREAM QUALITY ROUTING MODEL — QUAL2E INPUT DATA CODING FORMS

FORM ⑳ of ㉔

DATA TYPE 11A POINT LOAD AND WITHDRAWAL - 2

DATA TYPE	ORDER OF LOAD	ANC	COLI (NO / 100 MI)	CHL A (μG/L)	ORG N (MG/L)	NH3 N (MG/L)	NO2 N (MG/L)	NO3-N (MG/L)	ORG P (MG/L)	DIS P (MG/L)	(not used)
POINTLD 2 PTL*											
POINTLD 2 PTL*											
ENDATA11A											

FORMAT (2A4 A2 5X F5.0 9F6.0)

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ㉑ of ㉔

DATA TYPE 12 DAM REAERATION COEFFICIENTS

DATA TYPE	DAM NO	RCH NO OF DAM	ELE NO BELOW DAM	ADAM	BDAM	FRACTION FLOW OVER DAM FDAM	HEIGHT OF DAM HDAM (FT, M)	
DAM DATA DAM								
DAM DATA DAM ENDATA12								

FORMAT (3A4 A2 5X F5.0 6F6.0)

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ㉒ of ㉔

DATA TYPE 13 DOWNSTREAM BOUNDARY-1

DATA TYPE	TEMP (F, C)	DISSOLVED OXYGEN (MG/L)	BOD (MG/L)	CONS 1	CONS 2	CONS 3	ANC	COLIFORM (NO / 100 ML)
DOWNSTREAM BOUNDARY-1								
ENDATA13								

DATA TYPE 13A DOWNSTREAM BOUNDARY-2

DATA TYPE	CHL A (µG/L)	ORG N (MG/L)	NH3 N (MG/L)	NO2 N (MG/L)	NO3 - N (MG/L)	ORG P (MG/L)	DIS P (MG/L)	(not used)
DOWNSTREAM BOUNDARY-2								
ENDATA13A								

FORMAT (6A4 8F7.0)

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ㉓ of ㉔

LOCAL CLIMATOLOGICAL DATA

DATA TYPE	MONTH, DAY AND YEAR	HOUR OF DAY	NET SOLAR RADIATION	CLOUDINESS	DRY BULB TEMP	WET BULB TEMP	BAROMETRIC PRESSURE	WIND SPEED
LOCAL CLIMATOLOGY								
LOCAL CLIMATOLOGY								

*Must be chronologically ordered FORMAT (30X F10 0 5F8 0)

Net solar radiation is not required if temperature is simulated but is only required for dynamic algae simulation when temperature is not simulated

VARIABLE	ENGLISH UNITS	METRIC UNITS
Net Solar Radiation (PAR)	BTU/ft² hr	Langleys/hr
Wetbulb Drybulb Temps	F	C
Barometric Pressure	in Hg	millibars
Wind Speed	ft/sec	m/sec

NOTE These data must appear in a separate input data file (FORTRAN unit number 2) if dynamic/diurnal temperature simulations are being performed See Section X Climatological Data

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM ㉑ of ㉔

DO AND BOD REACH PLOT DATA

DATA TYPE	REACH NUMBERS IN ORDER FOR PLOTTING													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
BEGIN RCH														
PLOT RCH														
BEGIN RCH														
PLOT RCH														

FORMAT (A4 6X I5), FORMAT (10X 14I5)

BEGIN RCH Id number of first reach in the plot

PLOT RCH Reach numbers in the proper order for plotting

NOTE Multiple plots are obtained by repeating the seq ence of BEGIN RCH and PLOT RCH information (see User's Manual for example)

Form (24A)

PLOT OBSERVED DISSOLVED OXYGEN DATA

DATA TYPE	RIVER LOCATION (MI/KM)	MINIMUM DO (MG/L)	AVERAGE DO (MG/L)	MAXIMUM DO (MG/L)	
DO TITLE					
NUM LOCS					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
NUM LOCS					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					
DO DATA					

FORMATS DO TITLE (20A4)
NUM LOCS (10X I4)
DO DATA (10X 4F 10 0)

Notes Observed DO DATA for multiple plots are input by repeating the sequence of NUM LOCS and DO DATA information
These data must appear in a separate data file (FORTRAN unit number 2) from the QUAL2E input data file

APPENDIX B
USER MANUAL FOR QUAL2E UNCAS

I Introduction

The following sections provide instructions for assembling the two application-specific input data files for an UNCAS simulation The first provides the general specifications for the uncertainty analysis to be performed and the second contains the input uncertainty information for each input variable

II General Specification File ****.DAT

This data file named and prepared by the user contains the general requirements for performing a QUAL2E UNCAS simulation This input data file consists of nine data types as follows

UNCAS Data Type	Description
1	Heading
2	System Title
3	Uncertainty Option
4	Input Condition
5	Intermediate Output
6	Output Variables
7	Output Locations
8	Input Variables
9	Ending

Data Types 1 through 7 are read by subroutine UNDATA whereas Types 8 and 9 are read by subroutines INSENS or IFOAMC as necessary In all UNCAS data types the first 30 columns contain default data type descriptive information (see UNCAS Input Coding Form)

A UNCAS Data Type 1 Heading

This data type is a default header line for the beginning of the UNCAS general specification file It consists of one line and is prepared in the following format

Entry _ Text	Position
UNCAS1___*HEADING___________*	Columns 1-30
*QUAL2E UNCERTAINTY ANALYSIS	Columns 31 57

Note The underscore _ indicates a space

B UNCAS Data Type 2 System Title

This data type contains a user supplied descriptive title (50 alphanumeric characters) for the uncertainty simulations It consists of one line and is formatted as follows

Entry	Position
"UNCAS2___*SYSTEM_TITLE_______*"	Columns 1-30
User Title	Columns 31-80

C UNCAS Data Type 3 Uncertainty Option

Data type 3 is where the user specifies the particular type of uncertainty analysis to be performed The descriptive text for this data type appears in the first 30 columns as follows

"UNCAS3___*UNCERTAINTY_OPTION-*"

There are three uncertainty options--sensitivity analysis first order error analysis and monte carlo simulation Also if first order or monte carlo are selected the user must supply the magnitude of the input pertubation or number of monte carlo simulations respectively Data type 3 consists of one line prepared with the descriptive text described above followed by one of these three options

Entry	Position
SENSITIVITY ANALYSIS	Columns 31-50
or	
"FIRST ORDER ERROR ANALYSIS "	Columns 31-57
Magnitude of input perturbation %*	Columns 59-64
" % PERTURBATION	Columns 66-79
or	
"MONTE CARLO SIMULATION "	Columns 31-53
Number of monte carlo simulations	Columns 59-64
"SIMULATIONS"	Columns 66-76

(* Enter as a percent If not specified a default value of 5% is used)

Note UNCAS tests the four alphanumeric characters in columns 31-34 (i e "SENS "FIRS or MONT") to determine the uncertainty analysis option desired

D UNCAS Data Type 4 - Input Condition

This data type provides UNCAS with information concerning the particulars of the inputs to be modified The 30 column descriptive text for this line of data is

UNCAS4___*INPUT_CONDITION____*"

If the sensitivity analysis option is being exercised data type 4 conveys to UNCAS whether the inputs (specified in Data Type 8) are to be perturbed (a) singly or in groups or (b) using a factorial design strategy For the factorial design option the user must specify the number of input variables in the design Currently UNCAS accommodates only 2 or 3 variable factorial designs For sensitivity analysis UNCAS data type 4 is completed with one of the following two selections

Entry	Position
SINGLE/MULTIPLE PERTURBATIONS"	Columns 31-59
or	
2 LEVEL FACTORIAL DESIGN	Columns 31 54
Number of input variables (2 or 3)	Column 63
VARIABLES	Columns 64 73

If the first order error analysis or the monte carlo simulation option is selected data type 4 is used to specify which of the generic groups of input variables are to be varied These groupings are defined according to the QUAL2E input data types and are specified using the following alphanumeric code

QUAL2E Input Variables	QUAL2E Data Types	UNCAS Alphanumeric Code
Global	1 1A 1B	GLBL
Hydraulic/Climatology	5 5A	HYDR
Reaction Coefficient	6 6A 6B	RXNC
Incremental Flow	8 8A	FTIF
Headwater Conditions	10 10A	FTHW
Point Loads	11 11A	FTPL
Dams	12	FTDM

For the first order and monte carlo options data type 4 is completed with one of the following two selections

Entry	Position
"ALL INPUTS	Columns 31-40
or	
"GENERIC GROUPS	Columns 31-44
1st alphanumeric code	Columns 47 50
2nd alphanumeric code	Columns 52 55
3rd alphanumeric code	Columns 57-60
4th alphanumeric code	Columns 62-65
5th alphanumeric code	Columns 67-70
6th alphanumeric code	Columns 72 75
7th alphanumeric code	Columns 77-80

Any number (from 1-7) of groups may be specified and only the QUAL2E inputs that (those) group(s) will be perturbed in the uncertainty analysis Note UNCAS tests the four alphanumeric characters in columns 31 34 (i e "SINGLE "ALL_ or "GENE") to determine the input condition desired

E UNCAS Data Type 5 Intermediate Output

With data type 5 the user can specify whether any intermediate output is desired Intermediate output is defined as line printer output for each uncertainty simulation The 30 column descriptive text for this line of data is

"UNCAS5___'INTERMED_OUTPUT____"

UNCAS recognizes three options for intermediate output none a complete QUAL2E final summary and a limited output summary The limited intermediate output summary consists of an echo print of the inputs that have been perturbed for the uncertainty simulation a summary of the steady state temperature and algae convergence computations and a tabulation of the base and new values of the output variables at the locations specified (UNCAS Data Type 7) Entries for data type 5 are completed with one of the following 3 selections

Entry	Position
"NONE	Columns 31 34
or	
COMPLETE QUAL2E FINAL SUMMARY	Columns 31 59
or	
'LIMITED	Columns 31 37

Note because of the potential for voluminous output the second and third options are not available for monte carlo simulation UNCAS tests the four alphanumeric characters in columns 31 34 (i e NONE COMP or LIMI) to determine the intermediate output desired

UNCAS Data Type 6 Output Variables

Data type 6 is used to constrain the list of output variables for which uncertainty results will be computed These constraints are applied in a manner analogous to the input variable constraints in data type 4 The user simply specifies the generic groups of output variables for which uncertainty results are desired The 30 column descriptive text for this line of data is

UNCAS5___*OUTPUT_VARIABLES___*

The generic output groups are named HYDRAULIC QUALITY AND 'INTERNAL The hydraulic group consists of 10 output variables (flow depth velocity dispersion etc) associated with the hydraulic output from QUAL2E The quality group consists of the values of the 17 state variables simulated by QUAL2E The internal group is made up of 9 diagnostic or internal variables associated with the algal nutrient light interactions in QUAL2E (i e algal growth rate p minus r and p/r ratio light and nutrient factors in the growth rate computation nitrification inhibition factor etc) This data type is completed by adding the names of the generic output variable groups to the data type 6 line as follows

Entry	Position
Generic Output Group 1	Columns 31 40
Generic Output Group 2	Columns 46-55
Generic Output Group 3	Columns 61 70

Note UNCAS tests the four alphanumeric characters in columns 31 34 46 49 and 61-64 (i e HYDR ' QUAL or INTE") to determine the generic group of output variables to be analyzed They may be placed in any order in the appropriate positions

C UNCAS Data Type 7 Output Locations

This data type is used to define the locations in the basin where the output variables are to be examined for uncertainty analysis The 30 column descriptive text for UNCAS data type 7 is

"UNCAS7___*OUTPUT_LOCATIONS___*"

UNCAS will accept a maximum of 5 locations in the basin for output analysis They are supplied as a single line in the form of reach and element number as follows

Entry	Position
Location 1 (Reach and Element Number)	Columns 33 35 36 38
Location 2 (Reach and Element Number)	Columns 41-43 44-46
Location 3 (Reach and Element Number)	Columns 49 51 52 54
Location 4 (Reach and Element Number)	Columns 57 59 60-62
Location 5 (Reach and Element Number)	Columns 65-67 68 70

Note Reach and element numbers must be right justified in their appropriate column fields

4 UNCAS Data Type 8 - Input Variables

This data type is used to supply UNCAS with the input variable specifications for performing sensitivity analysis It is not required for the first order error analysis and monte carlo simulation options The 30 column descriptive text for UNCAS data type 8 is

"UNCAS8___*INPUT_VARIABLES*"

This data type will consist of one or more lines depending on how many sensitivity simulations are desired and/or on how many variables are to be sensitized in a given simulation

The information in this data type is designed to handle any of three different input conditions for sensitivity analysis one variable at a time variables in groups or factorially designed The data on each line consists of specifying the input condition the number of variables to be sensitized the name of the input variable and the magnitude of the perturbation

For a one variable at a time simulation one line of input is required as follows

Entry	Position
"SINGLE"	Columns 31 36
Number of inputs perturbed	Column 45
Input variable code	Columns 48-56
Magnitude of perturbation %	Columns 58-63

The number of inputs perturbed with this option is always 1 The input variable codes are 8 alphanumeric characters as shown in Table B-1 This line of data may be repeated for one variable at a time sensitivity simulations with other variables or other levels of perturbation

For sensitivity analyses where more than one variable is perturbed one line of input is required for each input variable to be altered as follows

Entry	Position
"MULTIPLE"	Columns 31-38
Number of inputs perturbed	Column 45
Input variable code	Columns 49-56
Magnitude of perturbation	Columns 58 63

UNCAS limits the number of inputs perturbed for this option to be either 2 or 3 thus requiring 2 or 3 lines of UNCAS data type 8 respectively The input variable codes are shown in Table B 1 As with one variable at a time simulations groups of multiple variable sensitivity simulations may appear one after the other in this data type

For sensitivity analysis using variables in a factorically designed configuration one line of input is required for each input variable as follows

Entry	Position
"FACTORIAL	Columns 31 39
Number of Inputs perturbed	Column 45
Input variable code	Columns 49 56
Magnitude of perturbation %	Columns 58 63

UNCAS limits the number of inputs perturbed in the factorial design optio to be either 2 or 3 thus requiring 2 or 3 lines of UNCAS data type 8 respectively The input variable codes are shown in Table B 1 UNCAS automatically sets up conditions for each of the 4 or 8 factorial design simulations As with the other sensitivity analysis options groups of factorial design conditions may appear one after the other in this data type

Note UNCAS tests the four alphanumeric characters in column 31 34 (i e SINC "MULT and FACT) to determine the sensitivity analysis option desired UNCAS also allows the user to mix the sensitivity analysis option types in a single execution of the program however the maximum number of sensitivity simulations is 120 This data type is not required for the first order error analysis or monte carlo simulation options

I UNCAS Data Type 9 - Ending

This data type is a default ending line that signifies the end of the general specification file It consists of one line and is prepared in the following format

Entry Text	Position
UNCAS9___*ENDING_____________*	Columns 1 30
ENDUNCERTAINTY"	Columns 31-44

II Input Variance Data File INVAR DAT

This data file contains the uncertainty information for each input variable in QUAL2E An example of this file containing a set of default data is provided with the UNCAS package However the user must adjust the default data to values suitable for the particular case being modeled The data contained in INVAR DAT consists of the variable code name its QUAL2E data type its coefficient of variation and its probability density function The first two lines of the file are title and header lines Subsequent lines contain the variance information formatted as follows

Entry	Position
Input Variable Name	Columns 3-30
Input Variable Code	Columns 36 43
QUAL2E Data Type	Columns 49-50
Coefficient of Variation	Columns 56-60
Probability Density Function	Columns 68-69

The input variable codes are shown in Table 3 1 The two character codes for probability density function are "NM" for normal distribution and "LN" for log normal

TABLE B-1 INPUT VARIABLE NAME CODES

Input variable Name	Input Code	QUAL2E Data Type
Evaporation coef - AE	ECOEF-AE	1
Evaporation coef BE	ECOEF-BE	1
Oxygen uptake by NH3 oxdtn	NH3OXYUP	1A
Oxygen uptake by NO2 oxdtn	NO2OXYUP	1A
Oxygen prod by algae grwtn	AGYOXYPR	1A
Oxygen uptake by algy resp	AGYOXYUP	1A
Nitrogen content of algae	AGYNCON	1A
Phosphorus content of algy	AGYPCON	1A
Algy max spec growth rate	AGYGROMX	1A
Algae respiration rate	AGYRESPR	1A
Nitrogen half sat'n coef	NHALFSAT	1A
Phosphorus half sat'n coef	PHALFSAT	1A
Linear alg self shade coef	AGYEXTLN	1A
Non lin alg self shade co	AGYEXTNL	1A
Light sat'n coefficient	LSATCOEF	1A
Light averaging factor	LAVGFACT	1A
Number of daylight hours	NUMBDLH	1A
Total daily solar radt'n	TDYSOLAR	1A
Alg pref for ammonia-N	APREFNH3	1A
Alg to temp solar factor	A/TFACT	1A
Nitrification inhib fact	NHIBFACT	1A
5-D to ult BOD conv k-cof	5TOUBODK	1
Temp coef BOD decay	TC/BODDC	1B
Temp coef BOD settling	TC/BODST	1B
Temp coef O2 reaeration	TC/REAER	1B
Temp coef sed O2 demand	TC/SOD	1B
Temp coef organic-N decay	TC/NH2DC	1B
Temp coef organic-N set	TC/NH2ST	1B
Temp coef ammonia decay	TC/NH3DC	1B
Temp coef ammonia srce	TC/NH3SC	1B
Temp coef nitrite decay	TC/NO2DC	1B
Temp coef organic-P decay	TC/PRGDC	1B
Temp coef organic P set	TC/PRGST	1B
Temp coef diss-P source	TC/PO4SC	1B
Temp coef algy growth	TC/ALGRO	1B
Temp coef algy respr	TC/ALRES	1B
Temp coef algy settling	TC/ALSET	1B
Temp coef coli decay	TC/CLIDC	1B
Temp coef ANC decay	TC/ANCDC	1B
Temp coef ANC settling	TC/ANCST	1B
Temp coef ANC source	TC/ANCSC	1B
Daily averaging option	DIURNOPT	1A
Light function option	LFNOPTN	1A
Algae growth calc option	AGYGROPT	1A

Table B-1 (continued)

Input Variable Name	Input Code	QUAL2E Data Type
Dispersion corr constant	DISPSN-K	5
Coef on flow for velocity	COEFQV A	5
Expo on flow for velocity	EXPOQV B	5
Coef on flow for depth	COEFQH-C	5
Expo on flow for depth	EXPOQH-D	5
Manning's roughness n	MANNINGS	5
Side slope 1	TRAP SS1	5
Side slope 2	TRAP SS2	5
Bottom width	TRAP WTH	5
Slope of channel	TRAP SLP	5
Mean elevation of reach	ELEVATIN	5A
Dust attenuation coef	DUSTATTN	5A
Fraction of cloudiness	CLOUD	5A
Dry bulb air temperature	DRYBULB	5A
Wet bulb air temperature	WETBULB	5A
Barometric pressure	ATMPRES	5A
Wind speed	WINDVEL	5A
CBOD oxidation rate	BOD DECA	6
CBOD settling rate	BOD SETT	6
SOD uptake rate	SOD RATE	6
Reaeration rate option 1	K2 OPT1	6
Coef on flow for K2 opt-7	CQK2 OP7	6
Expo on flow for K2 opt 7	EQK2 OP7	6
Coef for K2 (TSIV) opt 8	K2COEF-8	6
Slope for K2(TSIV) opt 8	K2SLOP 8	6
Organic N hydrolysis rate	NH2 DECA	6A
Organic-N settling rate	NH2 SETT	6A
Ammonia-N decay rate	NH3 DECA	6A
Ammonia-N benthal source	NH3 SRCE	6A
Nitrite-N decay rate	NO2 DECA	6A
Organic P hydrolysis rate	PORG DEC	6A
Organic P settling rate	PORG SET	6A
Dissolved-P Benthal srce	DISP SRC	6A
Chla to algae ratio	CHLA/ART	6B
Algae settling rate	ALG SETT	6B
Light ext coefficient	LTEXTNCO	6B
Coliform decay rate	COLI DEC	6B
ANC decay rate	ANC DECA	6B
ANC settling rate	ANC SETT	6B
Initial temperature	INITTEMP	7A
Reaeration equation opt	K2OPTION	6
Incremental flow	INCRFLOW	8
Incr temperature	INCRTEMP	8
Incr dissolved oxygen	INCRDO	8

Table B.1 (continued)

Input Variable Name	Input Code	QUAL2E Data Type
Incr BOD	INCRBOD	8
Incr-consv min 1	INCRCM1	8
Incr-consv min 2	INCRCM2	8
Incr consv min 3	INCRCM3	8
Incr arbitrary non-cons	INCRANC	8
Incr-coliform	INCRCOLI	8
Incr algae	INCRCHLA	8A
Incr-organic-N	INCRNH2N	8A
Incr ammonia-N	INCRNH3N	8A
Incr-nitrite-N	INCRNO2N	8A
Incr-nitrate N	INCRNO3N	8A
Incr-organic-phos	INCRPORG	8A
Incr-dissolved phos	INCRDISP	8A
headwater flow	HWTRFLOW	10
Hwtr temperature	HWTRTEMP	10
Hwtr-dissolved oxygen	HWTRDO	10
Hwtr-BOD	HWTRBOD	10
Hwtr consv min 1	HWTRCM1	10
Hwtr consv min 2	HWTRCM2	10
Hwtr-consv min 3	HWTRCM3	10
Hwtr arbitrary non-cons	HWTRANC	10A
Hwtr-coliform	HWTRCOLI	10A
Hwtr algae	HWTRCHLA	10A
Hwtr organic N	HWTRNH2N	10A
Hwtr ammonia N	HWTRNH3N	10A
Hwtr-nitrite N	HWTRNO2N	10A
Hwtr nitrate N	HWTRNO3N	10A
Hwtr organic phos	HWTRPORG	10A
Hwtr dissolved phos	HWTRDISP	10A
Ptld trtmnt factor	PTLDTFCT	11
Point load flow	PTLDFLOW	11
Ptld temperature	PTLDTEMP	11
Ptld dissolved oxygen	PTLDDO	11
Ptld BOD	PTLDBOD	11
Ptld consv min 1	PTLDCM1	11
Ptld consv min 2	PTLDCM2	11
Ptld consv min 3	PTLDCM3	11
Ptld arbitrary non-cons	PTLDANC	11A
Ptld coliform	PTLDCOLI	11A
Ptld algae	PTLDCHLA	11A
Ptld-organic N	PTLDNH2N	11A
Ptld ammonia N	PTLDNH3N	11A
Ptld nitrite N	PTLDNO2N	11A
Ptld nitrate N	PTLDNO3N	11A
Ptld organic phos	PTLDPORG	11A
Ptld dissolved phos	PTLDDISP	11A
Dam coefficient a	DAMSACOF	12
Dam coefficient b	DAMSBCOF	12
Fraction of flow over dam	DAMSFRAC	12

QUAL2E UNCAS INPUT DATA CODING FORM GENERAL UNCAS SPECIFICATIONS

UNCAS DATA TYPE		INPUT DATA SHOWING OPTIONS (or) FOR DATA TYPES 3 4 5 AND 8
UNCA-1	HEADING	QUAL2E UNCERTAINTY ANALYSIS
UNCA-2	SYSTEM TITLE	
UNCA-3	UNCERTAINTY OPTION	SENSITIVITY ANALYSIS FIRST-ORDER ERROR ANALYSIS % PERTURBATION MONTE CARLO SIMULATION # SIMULATIONS
UNCA-4	INPUT CONDITION	SINGLE/MULTIPLE PERTURBATIONS 2-LEVEL FACTORIAL DESIGN VARIABLES GENERIC GROUPS ALL INPUTS
UNCA-5	INTERMED OUTPUT	NONE COMPLETE QUAL2E FINAL SUMMARY
UNCA-6	OUTPUT VARIABLES	
UNCA-7	OUTPUT	
UNCA-8	INPUT VARIABLE	SINGLE MULTIPLE FACTORIAL
UNCAS9	ENDING	ENDUNCERTAINTY

UNCAS1 (A4 1X I1)
UNCAS2 (A4 1X I1 24X 12A4 A2)
UNCAS3 (A4 1X I1 24X A4 24X F6 0)
UNCAS4 (A4 1X I1 24X A4 28X I1) or (A4 1X I1 24X A4 11X /(1X A4))
UNCAS5 (A4 1X I1 24X A4)
UNCAS6 (A4 1X I1 24X A4 3(A4 1 1X))
UNCAS7 (A4 1X I1 24X 5(2X 2F3 0))
UNCAS8 (A4 1X I1 24X A4 10X I1 3X 2A4 IX F6 0)

Notes

1 All data types consist of 1 line except UNCAS8 which may have more than one

2 Blank lines between data types shown here for clarity Actual input data file has no blank lines

APPENDIX C

QUAL2E-UNCAS Example Application

A Introduction

The material in this appendix provides an example of how the uncertainty methodologies in QUAL2E-UNCAS can be applied to a QUAL2E data set The sole purpose of this section is to demonstrate the utility of uncertainty analysis rather than to provide a definitive analysis of the river system from which the data were obtained The example input data files and some of the output data files that were used in this application are provided with the model code distributed by the Center for Water Quality Modeling (CWQM)

B Withlacoochee River Basin

The data used to demonstrate the capabilities of QUAL2E-UNCAS were obtained from a USEPA survey of the Withlacoochee River during October 1984 (Koenig, 1986) In this study, water quality simulations were examined for portions of the river subjected to both municipal and industrial waste loads In addition there is a significant accretion of flow from groundwater inputs The river has a uniform low slope, but is characterized by alternating shoals and pools (often in excess of 25 feet deep) Average depths during the survey periods were 5 2 to 14 8 feet, widths were 90 to 140 feet, and flows varied from 150 cfs at the headwater to 660 cfs at the end of the system Water quality is affected by algal activity resulting from municipal waste discharges above the section of stream studied The addition of industrial waste at RM 24, however, dramatically reduces light penetration to the extent that the algal population diminishes in the downstream direction

A location map of the basin is shown in Figure C-1 and a plot of observed and modeled dissolved oxygen concentrations is presented in Figure C-2 Ten state variables were simulated in this study, temperature, dissolved oxygen, carbonaceous BOD, four nitrogen forms, (organic, ammonia, nitrite, and nitrate), two phosphorus forms, (organic and dissolved), and algae as chlorophyll a A summary of the calibrated inputs and their variance estimates for the uncertainty analysis is shown in Table C-1 The calibrated values in general were obtained by adjusting field or laboratory measurements of the specific model inputs The variance estimates were computed from replicate data taken during the survey period and by inference from other published data (McCutcheon, 1985 and Bowie et al , 1985)

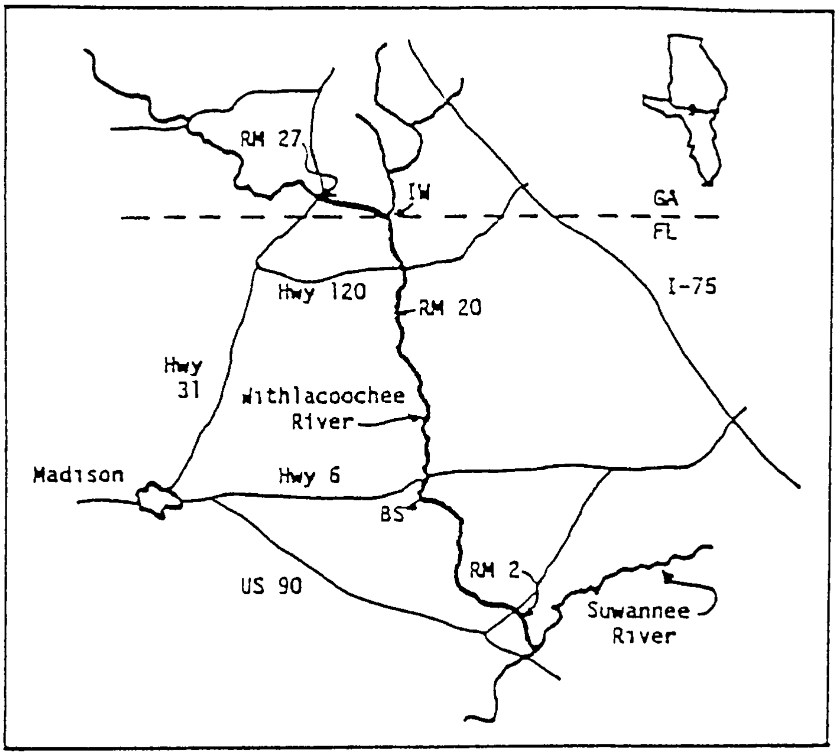


Fig C-1 Location map of the Withlacoochee River basin

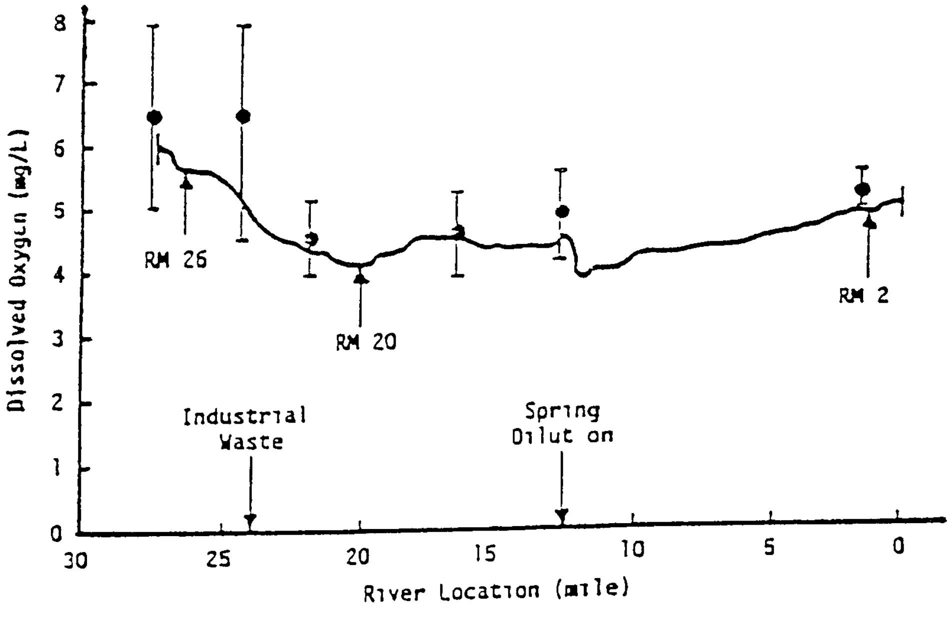


Fig C-2 Observed and predicted dissolved oxygen concentrations

C First Order Error Analysis (FOEA)

Table C-2 shows the first order error analysis (FOEA) results for the output variables of CBOD and DO at three locations in the Withlacoochee system an upstream location (RM 26), a midpoint near the dissolved oxygen sag (RM 20), and a downstream location (RM 2) For the CBOD sensitivity coefficients in Table C-2a, it is clear that the input forcing functions dominate model sensitivity In general, point load and headwater flows and CBOD have the largest sensitivity coefficients, however, their effects change with location in the system Headwater inputs dominate sensitivity in the upper reaches of the river and decrease in importance as one

TABLE C-1 Summary of Input Data for QUAL2E-UNCAS Simulations - Withlacoochee River Survey 1984

Input Parameter or Coefficient	Base Case (Mean) Values	Relative Standard Deviations (%)
Hydraulic Data (7)*		
Flows (cfs)	150 - 660	3%
Depths (ft)	5 2 - 14 8	8%
Velocities (fps)	12 - 78	8%
Others	a,b	10 - 20%
Reaction Coefficients (8)		
CBOD Decay (1/day)	04 - 10	15%
Reaeration (1/day)	08 - 80	13%
SOD (gm/ft^2-day)	04 - 13	12%
N, P, Algae	a,b	15 - 25%
Algae, Nutrient, Light Coefficients (17)		
Maximum Growth Rate (1/day)	1 3	10%
Respiration Rate (1/day)	15	10%
Others	a,b	10%
Climatology, Temperature inputs (23)		
Wet, Dry Bulb Air Temps (°F)	64 3, 74 5	2%
Temperature Coefficients	1 00 - 1 083	3%
Others	a,b	1 - 15%
Headwater, Incremental, Point Loads (27)		
DO, Temperature	a	1 - 3%
CBOD, N, P, Algae	a	8 - 25%

(a) Basin specific values from Koenig, 1986
(b) Typical values from Table III-3 of this report

* Value in parentheses is the number input variables of the type indicated

TABLE C-2 Summary of First Order Simulations for Withlacoochee River

(a) Simulation Variable CBOD

Input Variable	Relative Std Dev (%)	Sensitivity Coefficients RM 26	RM 20	RM 2	Components of Variance (%) RM 26	RM 20	RM 2
CBOD Decay	15	- 06 (3)*	- 11	- 22	1	2	8
Incr Flow	3	- 05	- 22	- 37 (3)	1	1	1
HW Flow	3	05	- 44 (3)	- 05	1	1	1
HW Temp	1	- 11 (2)	- 13	- 16	1	1	1
HW CBOD	15	98 (1)	24	18	99	9	6
Ptld Flow	3	00	67 (2)	43 (2)	0	3	1
Ptld CBOD	15	00	74 (1)	69 (1)	0	84	79
	Standard Deviation of Simulated CBOD (mg/L)				0 35	0 76	0 27
				(%)	15	12	12

(b) Simulation Variable Dissolved Oxygen

Input Variable	Relative Std Dev (%)	Sensitivity Coefficients RM 26	RM 20	RM 2	Components of Variance (%) RM 26	RM 20	RM 2
Velocity	8	03	05	- 26 (2)	1	2	13
CBOD Decay	15	- 02	- 12	- 03	1	9	1
SOD	5	- 05 (3)	- 23	09	5	20	3
Reaeration	13	04	31 (3)	40 (1)	4	45	77
Incr Temp	1	- 01	- 15	- 17 (3)	1	1	1
HW Temp	1	- 25 (2)	- 70 (1)	- 13	1	1	1
HW DO	3	92 (1)	55 (2)	04	84	8	1
	Standard Deviation of Simulated DO (mg/L)				0 18	0 27	0 30
				(%)	3	6	6

*( ) = rank with 1 being highest

proceeds downstream At the downstream location, the sensivity of CBOD to point load and incremental flow inputs is strong The sensitivity to the biochemical reaction coefficient grows in magnitude in the direction of flow, but is substantially smaller than the values associated with the point load forcing functions

Table C-2a also presents the components of variance for the modeled CBOD output These results show a similar, but somewhat modified pattern as the sensitivity coefficients The headwater CBOD is the dominant contributor (99%) to CBOD variability in the upper reaches of the basin The point load CBOD values are the primary variance component elsewhere in the river (84% at RM 20 and 79% at RM 2) The variance contribution from the CBOD rate coefficient grows in importance as one proceeds downstream, but is at least an order of magnitude lower than that from the CBOD point loads In the downstream portion of the basin, the variance contributions from the headwater inputs are small, as one would expect It is interesting to note that although the hydraulic inputs (incremental, point load, and headwater flow) have sensitivity coefficients that rank high, their contribution to CBOD variance is low because the relative standard deviation of these inputs is low (3%) compared to the CBOD loads (15%) The sensitivity coefficients and components of variance results at the sag point (RM 20) clearly show the upstream to downstream transition of the dominant input components The total variability in simulated CBOD estimated by the first order analysis, when expressed as a standard deviation, varies from 0 35 mg/L to 0 76 mg/L to 0 27 mg/L as one proceeds through the basin This prediction error is approximately 15% and is comparable to the magnitude of the error in the CBOD input forcing functions

The FOEA results for dissolved oxygen are presented in Table C-2b As contrasted with CBOD, the only forcing functions having large DO sensitivity coefficients are the headwater inputs, not the point load inputs Furthermore, DO is much more sensitive to temperature inputs than is CBOD As with CBOD, practically all the DO sensitivity in the upper reaches can be attributed to headwater DO however as one proceeds downstream, DO loses sensitivity to the headwater condition Next in importance in terms of DO sensitivity are the reaeration rate coefficient and velocity, both characteristic of system hydraulics The biochemical factors of sediment oxygen demand and CBOD rate coefficient follow in rank

Similar patterns of dissolved oxygen sensitivity are apparent from examining the components of variance (Table C-2b) The importance of reaeration and SOD is striking as is the relatively small impact of CBOD decay The temperature inputs, while having large sensitivity coefficients, provide a minimum contribution to DO variance Although algae dynamics were simulated in this application, their effect on DO uncertainty was negligible both in terms of sensitivity coefficient and components of variance The total variability in simulated DO when expressed as a standard deviation increases in the downstream direction varying from 0 18 mg/L to 0 30 mg/L and averaging about 5% of the simulated DO

D Effect of Model Non-linearity

First order error analysis uses the linear approximation to compute an estimate of output variance The validity of that approximation can be assessed by computing the sensitivity coefficients for both large and small values of ΔX, the input perturbation (see Eq VI-2) Small changes in the normalized sensitivity coefficient indicate near linearity of the state variable over the range of perturbed input values, whereas large changes in sensitivity reflect important nonlinear effects Table C-3 contains values of the normalized sensitivity coefficients for the state variables DO and chlorophyll a for input pertubations, ΔX, ranging from -20 to +20 percent The input variables selected for analysis are those having the largest sensitivity coefficients

For dissolved oxygen (Table C-3a), the reaeration and headwater temperature inputs show the largest relative changes in sensitivity, indicating that these variables have the largest nonlinear effects on DO The relative changes in sensitivity coefficient for the two inputs, however, are only 9 and 16%, respectively, suggesting that the nonlinear effects are not

TABLE C-3 Normalized Sensitivity Coefficients for Various Sizes of Input Perturbations (Withlacoochee RM 20)

(a) Simulation Variable Dissolved Oxygen (ug/L)

Input Variable	Magnitude of Input Perturbation % -20%	-1%	-1%	+20%	Relative Change (%)
CBOD Decay	- 12	- 12	- 12	- 12	0
SOD	- 23	- 23	- 22	- 23	0
Reaeration	33	31	31	30	-9
HW Temp	- 66	- 69	- 70	- 77	+16
HW DO	55	55	55	55	0
Std Dev (mg/L)	28	27	27	26	-7

(b) Simulation Variable (Chlorophyll a (ug/L)

Input Variable	-20%	-1%	-1%	+20%	Relative Change (%)
Max Growth Rate	40	41	42	43	+7
Respiration	- 37	- 36	- 35	- 34	-8
Chl a/Agy-B	-1 24	-1 01	- 98	- 83	-33
HW Flow	28	24	25	21	-25
HW Chl a	96	95	96	94	-2
Std Dev (ug/L)	3 72	3 12	3 06	2 64	-29

strong. The other three variables, CBOD decay, SOD, and headwater DO have normalized sensitivity coefficients that are essentially constant. Thus their impacts are, for practical purposes, linear for the conditions of this simulation. The net effect from all model input nonlinearities is manifest in the FOEA estimate of dissolved oxygen standard deviation, which decreases by 7% as the magnitude of the input perturbation changes fom -20 to +20 percent.

Similar, but more pronounced patterns are observed for the state variable, chlorophyll *a* (Table C-3b). Two input variables, the ratio of chlorophyll *a* to algal biomass (Chl*a*/Agy-B) and headwater flow exhibit large nonlinear effects on chlorophyll *a*. The maximum algal growth rate and the algal respiration rate show modest nonlinearities in sensitivity, while sensitivity to headwater chlorophyll *a* is essentially constant. The net FOEA estimate of standard deviation of chlorophyll *a* decreases by 29% over the range of input perturbations. Thus the effects of model nonlinearities appear to be stronger with chlorophyll *a* than with dissolved oxygen.

Analysis of other state variables showed changes in FOEA estimates of standard deviation of about 7% for algal growth rate, 5% for temperature and less than 5% for all others, including CBOD, the nitrogen forms and the phosphorus forms (see Table C-5). Note that, in all cases, the FOEA estimate of standard deviation decreases as the magnitude of the input perturbation increases over the range of -20 to +20%. It is curious that the large effect of model nonlinearities to chlorophyll *a* are not reflected in the dissolved oxygen sensitivites. This observation is perhaps explained by the fact that the largest input contributor to nonlinearity effects on chlorophyll *a* is a units conversion factor--the ratio of chlorophyll *a* to algal biomass. This factor does not serve as a linkage between the chlorophyll *a* and dissolved oxygen kinetic expressions in QUAL2E. The algal growth and respiration rates do provide that linkage, however, and the extent of their nonlinearities are comparable with that of dissolved oxygen, about 7%.

C Monte Carlo Simulations

The monte carlo simulation output in QUAL2E-UNCAS provides summary statistics and frequency distributions for the state variables at specific locations in the basin. Table C-4 contains the mean, minimum, maximuim, range, standard deviation, coefficient of variation, and skew coefficient for simulated dissolved oxygen and chlorophyll *a* at the upstream, midpoint, and downstream locations in the Withlacoochee basin. All summary statistics are based on 2000 monte carlo simulations using the same input variances that were employed in the first order error analysis. Input probability distributions were assumed to be normal.

There is very good agreement between the calibrated mean and simulated mean for dissolved oxygen. Differences are less than 0.5%. The differences between calibrated and simulated means for chlorophyll *a* average about 3% and may be attributed in part to the previously described nonlinearities in chlorophyll *a*. For dissolved oxygen, the standard deviation grows in the

TABLE C-4. Summary Statistics from 2000 Monte Carlo Simulations for Withlacoochee River

Statistic	Dissolved Oxygen (mg/L) RM 26	RM 20	RM 2	Chlorophyll a (ug/L) RM 26	RM 20	RM 2
Calibrated Mean	5.33	4.48	5.06	18.1	14.4	6.6
Simulated Mean	5.82	4.47	5.05	18.9	15.0	6.6
Minimum	5.26	3.47	3.69	10.2	2.8	3.0
Maximum	6.41	5.31	5.89	53.8	41.4	22.2
Range	1.15	1.84	2.20	45.6	33.6	19.2
Std. Deviation	0.18	.28	.31	4.25	3.48	1.87
Coef. Variation	3.0%	6.2%	6.2%	23.5%	24.2%	28.4%
Skew Coef	.01	-.15	-.20	1.73	1.60	1.46
Std. Deviation from FOEA	0.18	0.27	0.30	3.54	2.94	1.62

downstream direction. This phenomenon is attributable to the fact that dissolved oxygen never recovers to approach saturation (it lies in the 50 to 70% range) and to the cumulative effect of model input uncertainty as it propagates through the system. For chlorophyll a, the standard deviation decreases steadily in the downstream direction principally because the algal biomass concentration is also decreasing. The decrease in algal biomass concentration results from a lower algal growth rate attributable to reduced light penetration caused by color in the industrial waste discharge at RM 24 and to the dilution effects from groundwater inflow. The coefficient of variation for chlorophyll a averages about 25% throughout the basin, whereas that for dissolved oxygen is about 5%. The dissolved oxygen data exhibit little skew, but the chlorophyll a data show marked positive skewness.

Estimates of output variance by monte carlo simulation are not affected by model nonlinearities. Thus a comparison of monte carlo generated standard deviations with those produced by first order error analysis should provide information on the extent of any nonlinearities. As shown in Table C-4, these two estimates differ by less than 5% for DO and by about 20% for chlorophyll a. This comparison indicates weak nonlinearities associated with dissolved oxygen and more substantial ones with chlorophyll a, thus supporting the previous sensitivity coefficient observations in the first order error analysis. As shown in Table C-5, for the output variables of temperature, CBOD, and algal growth rate, the monte carlo estimate of standard deviation differs by less than 5% from the FOEA estimate. These differences are within the 95% confidence interval for the monte carlo estimates, thus implying negligible nonlinear effects for the conditions of this simulation The frequency distributions for dissolved oxygen generated by the monte carlo analysis are shown graphically in Figure C-3 These distributions are useful in providing a visual representation of the distribution of model output at different locations in the system In the case of dissolved oxygen shown in Figure C-3, the distributions appear nearly symmetric and the dispersion in the upper reaches of the basin is substantially smaller than that in the middle and lower reaches Similar plots (not shown) for chlorophyll a data in Table C-4 clearly show the decreasing dispersion and pronounced positive skew in the simulated data

F Number of Monte Carlo Simulations

A number of experiments were performed with the Withlacoochee data set to determine the number of monte carlo simulations required to achieve a given precision in the computed standard deviation of each output state variable Twenty replicate sets of 25, 50, 100, 200, and 500 monte carlo simulations were conducted The approximte 95% confidence interval (based on the assumption of normality) was computed for each replicate set and then plotted versus the total number of simulations performed The results for dissolved oxygen and CBOD are presented in Figure C-4 The smooth curve represents an envelope for the upper limit of the 95% CI for simulated standard deviation from repeated monte carlo simulations For both DO and CBOD it can be seen that about 1000 simulations are required to estimate the output standard deviation to within 5% of the mean With this criterion as a goal, 2000 monte carlo simulations were conservatively and routinely performed for the preceding analyses

TABLE C-5 Differences in Standard Deviation Estimates for Output Variables - Withlacoochee River Survey - 1984

Output Variables	Between FOEA Input Perturbations from -20 to +20%	Between FOEA (5%) and Monte Carlo Simulations (2000)
Temperature	5 4	1 8 - 4 3
Dissolved Oxygen	7 7	0 6 - 4 5
CBOD	0 8	1 4 - 2 6
Nitrogen Forms	*	*
Phosphorus Forms	*	*
Chlorophyll a	29	16 - 21
Algal Growth Rate	6 9	2 - 4

*Expected values of standard deviations too small to compute meaningful relative differences, although values are certainly less than 10% and likely less than 5%

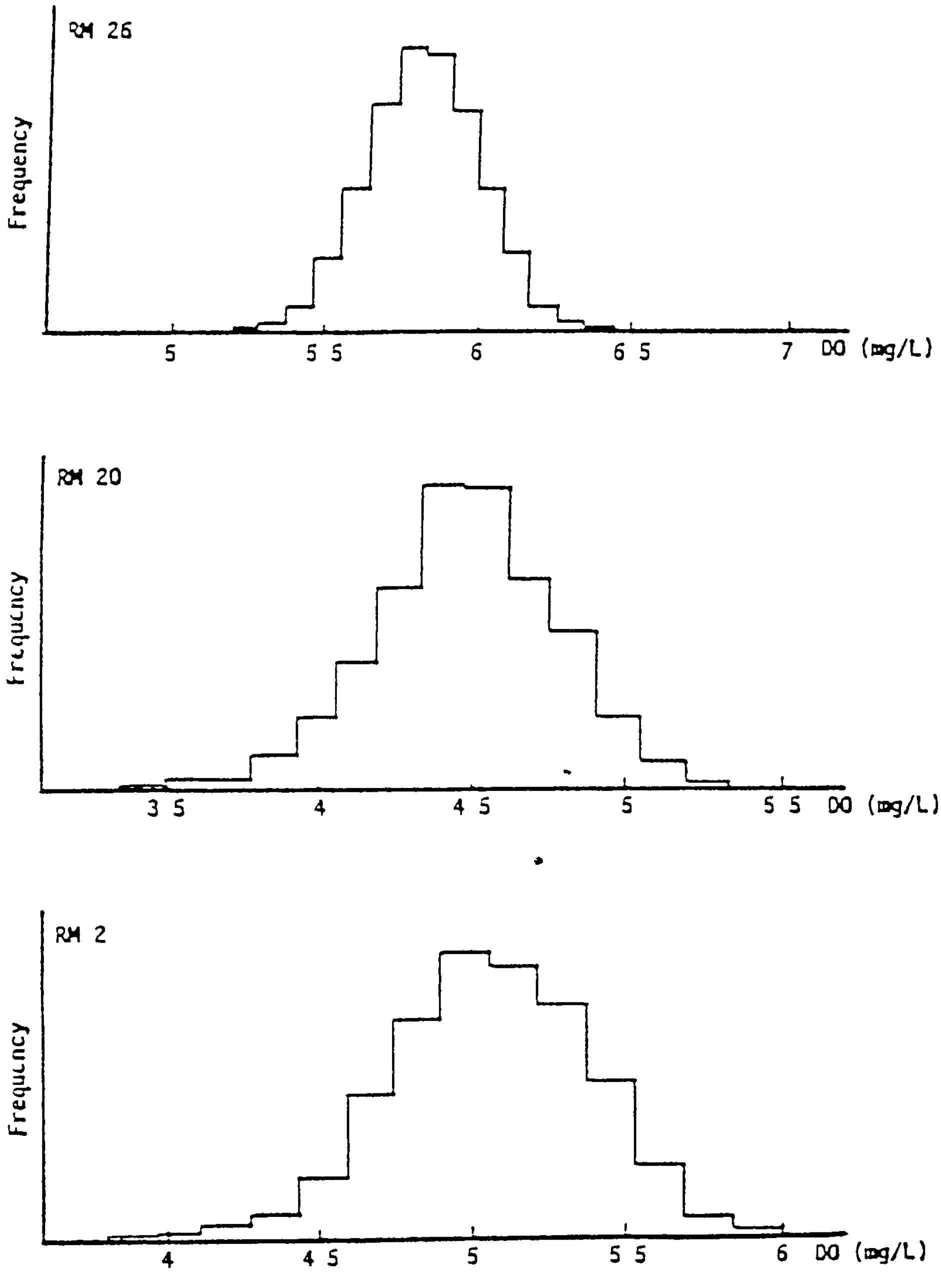


Fig C-3 Frequency distribution for dissolved oxygen from monte carlo simulations (Withlacoochee River)

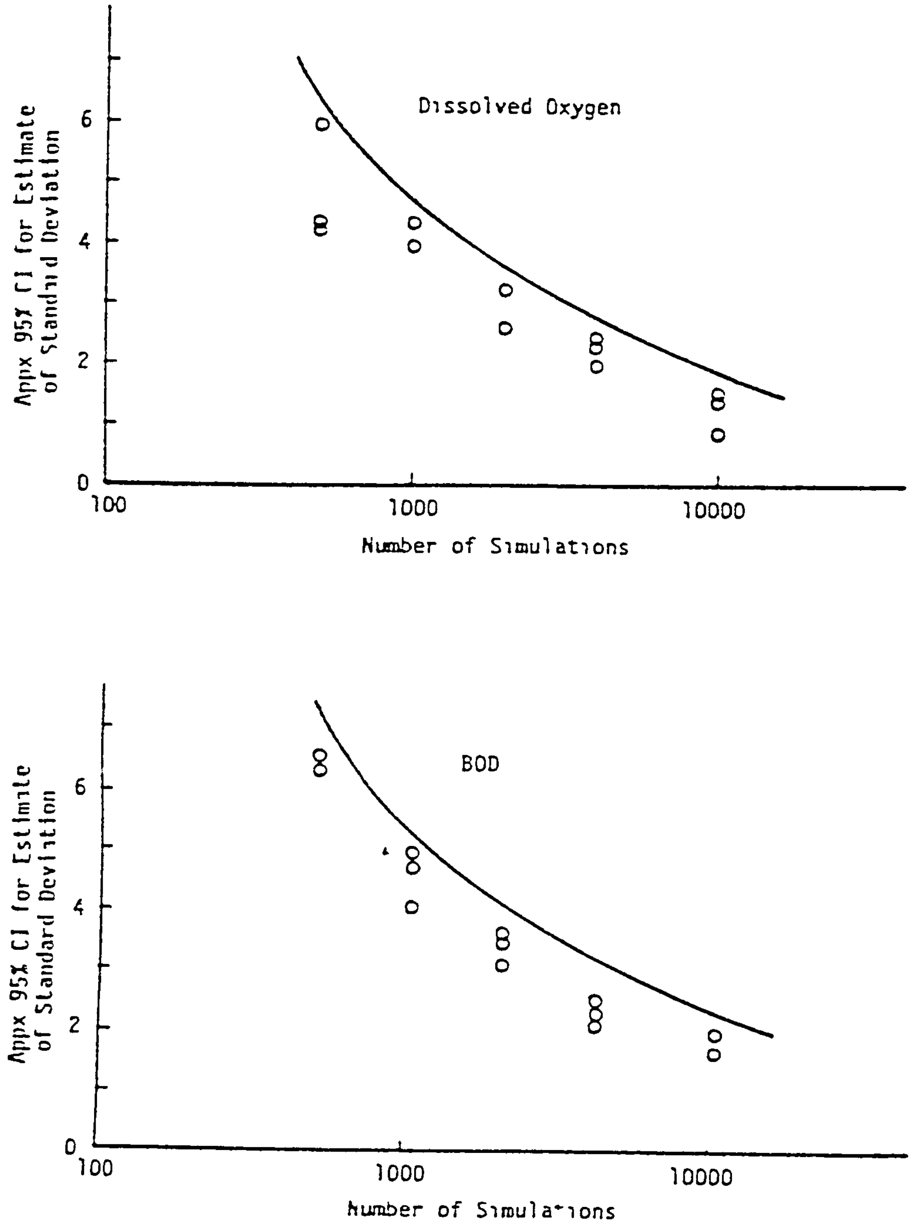


Fig C-4 Convergence characteristics of monte carlo simulations with QUAL2E-UNCAS (Withlacoochee River)

Summary

The following observations summarize experience to date with uncertainty analysis using QUAL2E QUAL2E-UNCAS has been shown to provide a useful framework for performing uncertainty analysis in steady state water quality modeling Application of the first order error analysis and monte carlo simulation methodologies to a data set from the Withlacoochee River Basin has highlighted some of the useful features of uncertainty analysis These include the changing sensitivities and components of variance in different portions of the river basin, the assessment of model nonlinearities, and the convergence characteristics of monte carlo methods Better understanding of input variance and probability density functions, model nonlinearities and input parameter correlations are needed for more confident application of these techniques An evaluation of the input factors which contribute the most to the level of uncertainty in an output variable will lead modelers in the direction of most efficient data gathering or research In this manner the modeler can assess the risk of imprecise forecasts and recommend measures for reducing the magnitude of that imprecision

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REFERENCES

American Public Health Association, Inc , Standard Methods for the Examination of Water and Wastewater, American Public Health Association, 1965 (12th edition), 1985 (16th edition)

Anderson, E R., Energy Budget Studies in Water Loss Investigations--Lake Hefner Studies, Technical Report, U S Geological Survey, Washington, DC, Prof Paper 269, 1954

Arden, B W and K N Astill, Numerical Algorithms Origins and Applications, Addison-Wesley, Reading, MA, 1970

Bannister, T T , "Production Equations in Terms of Chlorophyll Concentration, Quantun Yield, and Upper Limit to Production," Limnology and Oceanography, Vol 19, No 1, pp 1-12, January 1974

Bowie, G L , W B Mills, D B Porcella, C L Campbell, J R Pagenkopt, C L Rupp, K M Johnson, P W H Chan, and S A Gherini, Rates, Constants, and Kinetics Formulations in Surface Water Quality Modeling, 2nd ed , EPA/600/3-85/040, U S Environmental Protection Agency, Athens, GA, 1985

Box, G E P , W G Hunter, and J S Hunter, Statistics for Experimenters, Wiley, New York, NY, 1978

Brandes, R J and A B Stein, WREDUN Model Documentation Report, Water Resources Engineers, Inc , prepared for Texas Department of Water Resources, Construction Grants and Water Quality Planning Division, no date

Butts, T A and R L Evans, "Small Stream Channel Dam Aeration Characteristics", Journal Environmental Engineering Division, ASCE, Vol 109, No 3, pp 555-573, June 1983

Chen, C W and G T Orlob, Final Report Ecologic Simulation of Aquatic Environments, Water Resources Engineers, Inc , prepared for the Office of Water Resources Research, U S Department of the Interior, Washington, DC, October 1972

Churchill, M A , H L Elmore and P A Buckingham, "The Prediction of Stream Reaeration Rates," International Journal of Air and Water Pollution, Vo 6, pp 467-504, 1962

Davies, O L (ed), *The Design and Analysis of Industrial Experiments*, Hafner Publishing Company, New York, NY, 1967

DeGroot, W T , "Modelling the Multiple Nutrient Limitation of Algal Growth," *Ecological Modelling*, Vol 18, pp 99-119, 1983

Department of Scientific and Industrial Research (DSIR), *Effects of Polluting Discharges on the Thames Estuary*, Water Pollution Research Technical Paper No 11, Her Majesty's Stationery Office, London, 1964

Duke, J H , Jr , A E Johnson, and H O Andrews, "Verification and Sensitivity of the Unsteady Flow and Water Quality Model, WRECEV", Contract No 68-01-2620, U S Environmental Protection Agency, by Water Resources Engineers, Inc , Austin, TX, 1976

Duke, James H , Jr , *Provision of a Steady-State Version of the Stream Model, QUAL*, Water Resources Engineers, Inc , Austin, TX, prepared for the U S Environmental Protection Agency, Washington, DC, November 1973

Edinger, J E and J C Geyer, *Heat Exchange in the Environment*, Johns Hopkins Univ , Baltimore, MD, 1965

Elder, J W , "The Dispersion of a Marked Fluid in Turbulent Shear Flow," *Jour Fluid Mech* , Vol 5, Part 4, pp 544-560, May 1959

Field, S D and S W Effler, "Photosynthesis-Light Mathematical Formulations," *Journal of Environmental Engineering Division*, ASCE, Vol 108, No EE1, pp 199-203, February 1982

Field, S D and S W Effler, "Light-Productivity Model for Onondaga, N Y.," *Journal Environmental Engineering Division*, ASCE, Vol 109, No EE4, pp 830-844, August 1983

Fisher, H B , Discussion to "Time of Travel of Soluble Contaminants in Streams," by T J Buchanan, *Proc Sanitary Eng Div* , ASCE, v 6, 1964

Fisher, H B , E J List, R C Y Koh, J Imberger, N H Brooks, *Mixing in Inland and Coastal Waters*, Academic Press, New York, NY, 1979

Frank D Masch and Associates and the Texas Water Development Board, *Simulation of Water Quality in Streams and Canals, Theory and Description of the QUAL-I Mathematical Modeling System*, Report 128, the Texas Water Development Board, Austin, TX, May 1971

Henderson, F M , *Open Channel Flow*, Macmillan Co , New York, NY, 1966

JRB Associates, "Users Manual for Vermont QUAL-II Model," prepared for U S Environmental Protection Agency, Washington, DC, June 1983

Jassby, A D , and T Platt, "Mathematical Formulation of the Relationship Between Photosynthesis and Light for Phytoplankton," *Limnology and Oceanography*, Vol 21, No 4, July 1976, pp 540-547

Kennedy, M S and J M Bell, "The Effects of Advanced Wastewater Treatment on River Water Quality", *Journal Water Pollution Control Federation*, Vol. 58, No 12, pp 1138-1144, December, 1986

Koenig, M , Withlacoochee River - QUAL2E model calibration from Clyatville, GA to Ellaville, FL (in preparation), U S Environmental Protection Agency, Region IV, Environmental Services Division, Athens, GA, 1986

Kramer, P H , *A Search of the Literature for Data Pertaining to Bioenergetics and Population Dynamics of Freshwater Fishes*, Desert Biome Aquatic Program, Utah State University, Logan, UT, August 1970

Langbien, W B and W H Durum, *The Aeration Capacity of Streams*, U S Geological Survey, Washington, DC, Circ 542, 1967

Malone, R , D S Bowles, M P Windham, and W J Grenney, "Comparison of Techniques for Assessing Effects of Loading Uncertainty Upon a Long Term Phosphorus Model", *Applied Mathematical Modeling*, Vol 7, No 1, pp 11-18, Feb 1983

McCutcheon, S C , Water quality and streamflow data for the West Fork Trinity River in Fort Worth, TX, U S Geological Survey, *Water Resources Investigation Report 84-4330*, NTSL, MS, 1985

National Council for Air and Stream Improvement, Inc , *A study of the selection, calibration and verification of mathematical water quality models*, NCASI Technical Bulletin No 367, New York, NY, March 1982

National Council for Air and Stream Improvement, Inc , *A Review of the Mathematical Water Quality Model QUAL-II and Guidance for its Use*, NCASI, New York, NY, Technical Bulletin No 391, December 1982

National Council for Air and Stream Improvement, Inc , *QUAL2E User Manual*, NCASI, New York, NY, Technical Bulletin No 457, February 1985

O'Connor, D J and W E Dobbins, "Mechanism of Reaeration in Natural Streams, *Trans ASCE*, Vol 123, pp 641-684, 1958

O'Neill, R V , and R H Gardner, "Sources of Uncertainty in Ecological Models In B P Zeigler, M S Elzas, G L Klir, T I Oren, eds *Methodology in Systems Modelling and Simulation* North-Holland Publishing Co , New York, pp 447-463, 1979

Owens, M , P W Edwards and J W Gibbs, "Some Reaeration Studies in Streams," *International Journal of Air and Water Pollution*, Vol 8, No 8/9, pp 469-486, September 1964

Plate, E J (ed), Engineering Meteorology, Studies in Wind Engineering and Industrial Aerodynamics, Vol 1 Fundamentals of Meteorology and Their Application to Problems in Environmental and Civil Engineering, Elsevier Scientific Publishing Company, Amsterdam, 1982

Platt, T , K H Mann, and R E Ulanowicz (eds), Mathematical Models in Biological Oceanography, Unesco Press, Paris, 1981

Reckhow, K H , Quantitative Techniques for the Assessment of Lake Quality, U S Environmental Protection Agency, Washington, D C , EPA-440/5-79-015, 1979

Roesner, L A , Temperature Modeling in Streams, Lecture notes, water quality workshop, Tennessee Valley Authority, Knoxville, TN, 1969

Roesner, L A , P R Giguere, and D E Evenson, Computer Program Documentation for Stream Quality Modeling (QUAL-II) U S Environmental Protection Agency, Athens, GA, EPA-600/9-81-014, February 1981a

Roesner, L A , P R Giguere, and D E Evenson, User's Manual for Stream Quality Model (QUAL-II) U S Environmental Protection Agency, Athens, GA, EPA-600/9-81-015, February 1981b

Rose, K A , and G L Swartzman, "A Review of Parameter Sensitivity Methods Applicable to Ecosystem Models", Report NRC FIN B7018, prepared for the U S Nuclear Regulatory Commission, Washington, D C , May 1981

Scavia, D and R A Park, "Documentation of Selected Constructs and Parameter Values in the Aquatic Model CLEANER," Ecological Modeling, Vol 2, pp 33-58, 1976

Scavia, D , W F Powers, R P Canale, J L Moody, "Comparison of First-Order Error Analysis and Monte Carlo Simulation in Time-Dependent Lake Entrophication Models", Water Resources Research, Vol 17, No 4, pp 1051-1059, 1981

Smith, E L , "Photosynthesis in Relation to Light and Carbon Dioxide," Proceedings, National Academy of Sciences, Vol 22, pp 504-510, 1936

Smith, J D , Solutions to Partial Differential Equations, Macmillan Co , New York, NY, 1966

St John, J R , T W Gallagher, and P R Paquin, "The Sensitivity of the Dissolved Oxygen Balance to Predictive Reaeration Equations," in Gas Transfer at Water Surfaces, W Brutsaert and G Jirka, eds , D Reidl Publishing Company, Dordrecht, Holland, 1984

Steele, J H , "Environmental Control of Photosynthesis in the Sea," Limnology and Oceanography, Vol 7, pp 137-150, 1962

Stefan, H G , J J Cardoni, F R Schiebe, and C M Cooper, 'Model of Light Penetration in a Turbid Lake," Water Resources Research, Vol 19, No 1, pp 109-120, February 1983

Stone, H L and P O T Brian, "Numerical Solution of Convective Transport Problems," Journal American Institute of Chemical Engineers, Vol 9, No 5, pp 681-688, 1963

Streeter, H W and E B Phelps, Study of the Pollution and Natural Purification of the Ohio River, U S Public Health Service, Washington, DC, Bulletin No 146 (reprinted 1958), 1925

Swartzman, G L and R Bentley, "A Review and Comparison of Phytoplankton Simulation Models," Journal of the International Society for Ecological Modelling, Vol 1, Nos 1-2, pp 30-81, 1979

Taylor, G I , "The Dispersion of Matter in Turbulent Flow Through a Pipe," Proceedings Royal Society of London, Vol 234A, No 1199, pp 456-475, March 6, 1954

Texas Water Development Board, Simulation of Water Quality in Streams and Canals, Program Documentation and User's Manual, Austin, TX, September 1970

Texas Water Development Board, QUAL-TX Users Manual, Version 2 5, Water Quality Management Section Austin, TX, November 1984

TenEch Environmental Consultants, Inc Waste Load Allocation Verification Study Final Report Prepared for Iowa Department of Environmental Quality, July 1978

Thackston, E L and P A Krenkel, Reaeration Prediction in Natural Streams, Journal of the Sanitary Engineering Division, ASCE, Vol 95, No SA1, pp 65-94, February 1969

Thomas, H A , Jr , "Pollution Load Capacity of Streams " Water and Sewage Works, Vol 95, No 11, pp 409-413, November 1948

Tsivoglou, E C and J R Wallace, Characterization of Stream Reaeration Capacity, Prepared for U S Environmental Protection Agency, Washington, DC, 1972

Tsivoglou, E C and L A Neal, "Tracer Measurement of Reaeration III Predicting the Reaeration Capacity of Inland Streams," Jour WPCF, Vol 48, No 12, pp 2669-2689, December 1976

Walker, W W , QUAL2 Enhancements and Calibration to the Lower Winooski Prepared for the Vermont Agency of Environmental Conservation, Montpelier, VT, December 1981

Walker, W W , "A Sensitivity and Error Analysis Framework for Lake Entrophication Modeling", Water Resources Bulletin, Vol 18, No 1, pp 53-60, Feb 1982

Walker, W W Personal Communication, 1983

Water Resources Engineers, Inc , Prediction of Thermal Energy Distribution in Streams and Reservoirs, Prepared for the California Dept of Fish and Game, 1967

Water Resources Engineers, Inc Progress Report on Contract No 68-01-0713, Upper Mississippi River Basin Model Project, Sponsored by the Environmental Protection Agency, submitted to Environmental Protection Agency, September 21, 1972

Wunderlich, W O , The Fully-Mixed Stream Temperature Regime, ASCE Specialty Conf , Utah State Univ , Logan, Utah, 1969