

行政院及所屬各機關出國報告

(出國類別：考察)

美國清淨製程研究之發展現況考察報告

出國人：台灣大學化工系余政靖教授
中央大學化工系李亮三教授
中原大學化工系阮若屈教授
國家科學委員會工程技術發展處朱曉萍研究員

出國地區：美國

出國期間：90年9月3日至90年9月17日

報告日期：90年12月31日

行政院及所屬各機關出國報告

(出國類別： 考察)

美國清淨製程研究之發展現況考察報告

出國人：台灣大學化工系余政靖教授
中央大學化工系李亮三教授
中原大學化工系阮若屈教授
國家科學委員會工程技術發展處朱曉萍研究員

出國地區：美國

出國期間：90年9月3日至90年9月17日

報告日期：90年12月31日

摘要

基於環保需求及社會對產業永續發展之重視，清淨製程技術已成為本世紀一項重要之研究課題，其研究範疇涵蓋清潔生產、工業生態及污染防治等領域，目前國內已有多位學者投入相關領域之學術研究，研發能量已粗具規模，有待進一步之規劃及整合。基於此，化工學門邀請了學門召集人台大化工系余政靖教授、中原大學阮若屈教授、中央大學李亮三教授及選派工程處朱曉萍研究員組成考察團，赴美國卡內基美隆大學、俄亥俄州立大學、聖母大學及柏克萊大學等相關單位參訪，期能吸取國外在規劃及推動清淨製程研究和課程方面的經驗和心得，可做為未來國內推動相關課題時的重要參考。並順道參加國科會駐芝加哥科學組在美國所舉辦的中美雙邊 2001 CHEM TECH.研討會，以促進華人間之學術交流。

在參訪的過程中，每一個參訪單位皆很熱心的安排了相當緊湊的行程，並極力安排相關的研究學者與吾人共同討論，在熱烈互動的過程中，得以了解各單位在清淨製程方面的研究驅勢，及配套之課程安排，實在是獲益良多。

惟在考察行程中，不巧遇到美國境內發生 911 恐怖攻擊事件，致使原訂欲考察柏克萊大學的行程被迫取消，並在美國滯留五天，飽受精神威脅後，終能順利返國。由此次難得的經驗中亦感受到：美國雖為科技軍事強國，但似乎少有緊急應變處理的經驗，在面對突發的恐怖事件時，似顯得手足無措，以致遲遲無法妥善安排新的航空安檢措施。

綜而言之，經由這次的考察過程，吾人了解到了美國在清淨製程領域的研究方向、技術水準，以及美國學校在相關課程安排上的用心，這些都是我國日後值得參考和借鏡的地方。此外，吾人亦深刻體認到我國未來應規劃成立『綠色設計及製造中心』，並利用發展中的清淨製程相關技術與產業界進行技術交流，進行相關之專題研究計劃，以提供工業界設計方針與製造技術的支援，可考慮合作的主題包括：綠色設計相關的程序系統工程、綠色設計相關的基本製程技術及污染防治。

目次

	頁數
一、 考察目的-----	5
二、 考察成員-----	6
三、 考察行程-----	7
四、 考察過程及心得-----	8
五、 結語與建議-----	20
六、 附錄-----	22

一、 考察目的

基於環保需求及社會對產業永續發展之重視，清淨製程技術已成為本世紀一項重要之研究課題，其研究範疇涵蓋清潔生產、工業生態及污染防治等領域，目前國內已有多位學者投入相關領域之學術研究，研發能量已粗具規模，有待進一步之規劃及整合。基於此，化工學門邀請相關學者專家組成考察團，並選擇在清淨製程整體研究技術居領先地位的美國為參訪國家，同時經初步蒐集相關資訊後，進一步挑選在清淨製程方面著有聲名的相關實驗室做為參訪機構，分別為卡內基美隆大學、俄亥俄州立大學及聖母大學，期能吸取國外在規劃及推動清淨製程研究和設計課程方面的經驗和心得，以做為未來國內推動相關課題時的重要參考。

二、考察成員

本次考察成員共四人，分別為：
台灣大學化工系余政靖教授（化工學門召集人），
中央大學化工系李亮三教授，
中原大學化工系阮若屈教授，及
國科會工程處朱曉萍研究員（化工學門承辦人）。

三、考察行程

化工學門「清淨製程」技術發展考察小組實際行程

日期	住宿地點	工作紀要
9月3日(一)	舊金山	啟程赴美，等候轉機
9月4日(二)	匹茲堡	轉機赴賓州卡內基美隆大學
9月5日(三)	匹茲堡	訪問卡內基美隆大學 Green Design Center
9月6日(四)	Columbus	搭機前往俄亥俄州
9月7日(五)	Columbus	訪問俄亥俄州立大學化工系
9月8日(六)	芝加哥	參加中美雙邊研討會(2001 Chem Tech)
9月9日(日)	芝加哥	整理資料
9月10日(一)	芝加哥	訪問聖母大學 Environmentally Conscious Chemical Processes Design Lab
9月11-14日	芝加哥	美國發生 911 事件，取消所有航班
9月15日(三)	舊金山	由芝加哥搭機赴舊金山
9月16,17日	舊金山	搭機返台

四、考察過程及心得

(一)卡內基美隆大學綠色製造中心

1.背景介紹

卡內基美隆大學是相當具特色的一流私立大學，全校七千位學生中有 1/3 是研究生，工學院的設計研究中心(Engineering Design Research Center; EDRC)是美國國家科學基金會(NSF)最早成立的工程研究中心(Engineering Research Center; ERC)之一。此中心由十三個系所組成，在 1986-1997 年間，主要經費由美國國家科學基金會提供由最初的每年 400 萬美金，在四年後成長至每年 800 萬美金。這十一年的培育過程，卡內基美隆大學成長為最具競爭力的工程設計學校，但這成長並未因 NSF 經費終止而暫停。學校將 EDRC 轉型成複雜工程學院(Institute for Complex Engineered Systems; ICES)，此學院除了原本的 EDRC 外還加入如：Micro Electro-Mechanical Systems (MEMS)，Tissue Engineering and Artificial Organs 等九個子中心組成的機構。此學院著重與業界的合作且其參與方式分四級：Affiliate (\$25,000/年)，Member (\$60,000/年)，Partner (\$100,000~\$150,000/年)，Strategic Partner (\$200,000~\$300,000/年)(附錄一)。參與的好處由技術報告的取得至計畫合作到共同爭取政府計畫。簡單來說，這是一所素質高，企圖心強的私立大學，而事實也證明他們在工程研究上經營的非常成功。

2.訪問經過

整個訪問由上午 9 點進行至下午 4 點，而訪談的對象包括：A. Westrerberg, I. Grossmann, G. Powers, L. Biegler, E. Ydstie, S. Hauan 等六位教授及其學生。這六位教授有兩位是國家工程學院院士，兩位是重要期刊的副主編。剛開始我們花 20 分鐘介紹台灣化工研究現況及來訪目的，接下來每 50 分鐘分別由該系教授介紹他們的研究題目及成果。這六位教授的研究主題主要環繞在程序系統工程，主題包括設

計，最適化及控制，雖然領域接近，研究上的合作卻異常密切，這是相當難能可貴的。Westrerberg 主要研究在 conceptual design 及大型計算，Grossmann 是最適化的專家目前主要著重供給鏈管理，他也是首位將 mixed integer linear programming (MILP) 引入程序設計的研究者。Powers 較著重科技管理也大約略描述了 EDRC 和 ICES 的形成及目的。Biegler 也是動態最適化的專，研究著重動態系統集程序操作，因為他是目前化工系中的 Center for Advanced Process Decision-Making (CAPD) 的主任，他介紹了 CAPD 的概況(請參見附錄一)。CAPD 主要成員包括六位教授，三十位研究生及十二位博士後研究，每年經費約為 200 萬美金，其中 85% 來至國家科學基金會及能源部。他們也體認到程序系統工程的研究主題逐漸由設計轉向操作，研究內容也由工廠範疇擴大至商業範圍，這也是一個值得大家深思的議題。Ydstie 研究主題是控制領域涵蓋理論的適應控制到和 PPG 等公司合作的實際問題解決，Hauan 對高速計算(high performance computing) 相當有興趣但主要研究還是在反應蒸餾上，但對一位助理教授來說專長必須是全面的，所以也參與微系統，microbalance system 的開發。

3. 參訪心得

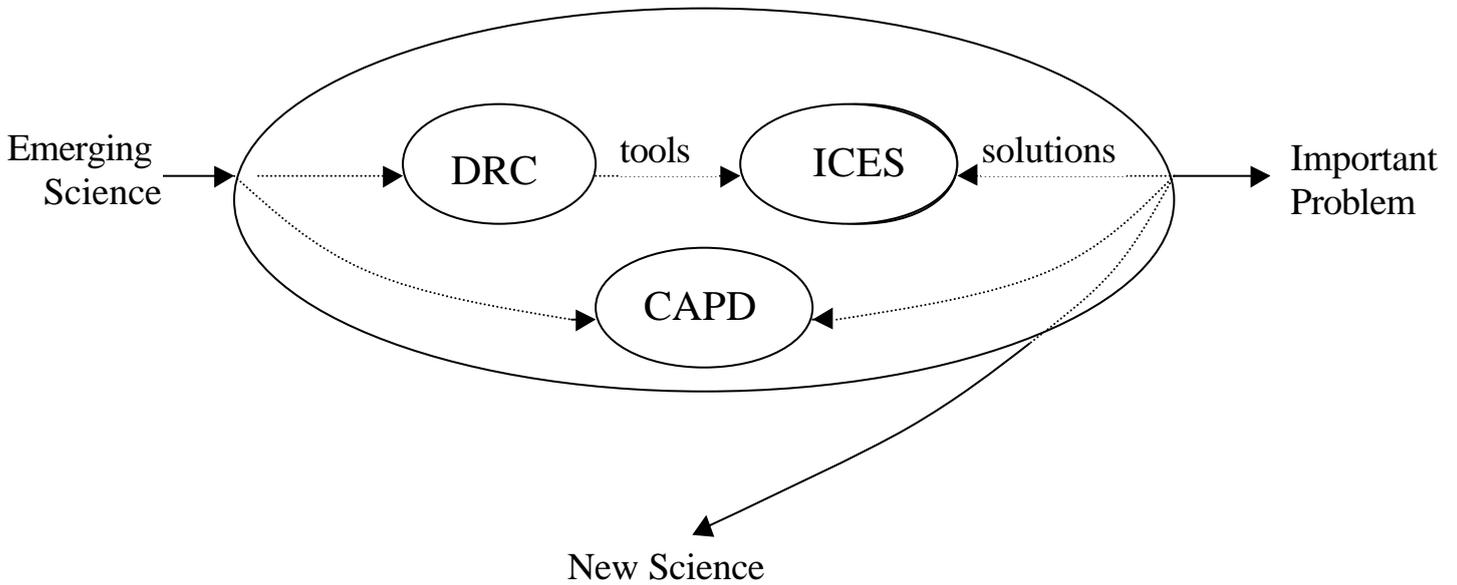
卡內基美隆大學的參訪讓我們體認到工程系所整合研究的重要性，從早期的 EDRC 到目前的 ICES，這些中心替卡內基美隆大學營造了一流大學的基石。但如何整合呢？以設計研究中心(EDRC)為例，首先我們必須了解設計的目的。

Design for:

- (1) Efficiency and Reliability
- (2) New Products
- (3) New Processes
- (4) Environment
- (5) Health and Safety

在確認目標後我們才能整合相關的系所及人才，如果產品是農業，醫藥，電子，高分子，則參與的人員都會有所不同。明確的目標是中心

成功的基本要素之一，接下來中心的定位為何？是先趨的開創者或者是實際問題的解決者？EDRC，CAPD 與 ICES 扮演了不同的角色。



上圖清楚的顯示 EDRC 扮演先趨的開創者的角色，ICES 扮演了實際問題的解決者的角色而 CAPD 較似兩者的混合體。所以目標，角色以及具體施行的決心才有可能促成一個成功的工程研究中心，這也是值得我們借鏡之處。

(二)俄亥俄州立大學化工系

1.背景介紹

俄亥俄州立大學化工系共有十三位全職服務的教員，一位榮譽教授，七十五位研究生及四百二十位大學生，與台灣的化工系相比，僅屬於中型規模。其主要之研究領域可概分為七項，而各領域之主要研究人員及研究主題如下：

(1)生物工程 / 生物技術

Jeffrey J. Chalmers - 生化工程、細胞培養、免疫磁性細胞分離

Shang-Tian Yang - 生化工程、醱酵、細胞培養、組織工程

Robert S. Brodkey - 人體大動脈系統中之流動量測

James F. Rathman - 生物系統中的界面現象

(2)膠體 / 粒子技術

Liang-Shih Fan - 粒體技術、流體化技術

James F. Rathman - 界面現象、分子自組、微胞催化、界面活性劑

Jacques L. Zakin - 界面溶液之流變學及微結構、減阻

David L. Tomasko - 以超臨界溶液形成粒子

Umit S. Ozkan - 多金屬奈米粒子的催化反應

(3)流體力學 / 多相流流動

Robert S. Brodkey - 混合及紊流流動、影像分析

Jeffrey J. Chalmers - 生化反應槽的攪拌現象及流體力學

Liang-Shih Fan - 流體化技術及多相流動力學

(4)分子熱力學 / 計算化學

Isamu Kusaka - 成核之理論和計算機模擬

David L. Tomasko - 超臨界流體熱力學、相平衡及分離

James F. Rathman - 溶液及界面中的分子自組現象

(5)高分子 / 複合材料加工

Kurt W. Koelling - 高分子加工、生物相容性聚合物、複合流體流變學

L. James Lee - 複合材料及高分子加工、反應性高分子、微製造技術

Robert S. Brodkey - 複合材料中的高分子孔隙結構成像

David L. Tomasko - 應用超臨界二氧化碳於高分子加工

(6)程序系統工程

Bhavik R. Bakshi - 化學整合製程操作、生態自覺製程設計

Martin Feinberg - 複雜反應系統的反應器最適化

(7)反應工程 / 催化反應

Martin Feinberg - 複雜反應動力學、化學反應網絡理論

Umit S. Ozkan - 雜相催化、觸媒的合成及特徵化

Liang-Shih Fan - 微粒之反應動力學

2.訪問經過

在 Ohio state university 的參訪中，我們拜訪了化工系、環工系及化學系的教授們，對「綠色製程」有了更深更廣的認識。

在 OSU 整天的行程中，由 Prof. Bhavik Bakshi 所安排。我們首先與化工系的 Prof. David Tomasko 會談，他研究的主題為超臨界 CO₂ 的應用，其中介紹了使用乾淨的 CO₂ 為溶劑，可以取代許多現在使用的有害溶劑，除了可使用超臨界 CO₂ 作為食品、藥品萃取的媒介，還將其應用於液相層析、高分子參合、製造發泡高分子。他並從事超臨界 CO₂ 與各種材料的介面現象的研究，一切為推廣清靜溶劑的努力，令人印象深刻。

接著我們拜訪了俄亥俄大學的環境分子科學中心(Environmental Molecular Science Center, EMSC)，會見了其副主席，化學系的 Prof. Patrick Hatcher，並參觀了該中心驚人的設備。OSU 之 Environmental Molecular Science Center，目的在以精密儀器測量污染物在氣相、液相、固相的分佈，藉此瞭解污染物在自然界自然代謝、自然傳輸的情況以及其與自然界其他物質間的物理、化學交互作用。他們擁有數套 GC-MS、LC-MS，並擁有高解析度之傅立葉轉換質譜儀、液相 NMR，及固相 NMR。Prof. Hatcher 原來在 Penn. State Univ.，被 OSU 以重金聘請，並提供一百萬美金購買這些儀器，也促使了環境分子科學中心的形成。此中心包括：環境系統工程、地質科學、環境工程及分析化學家十餘位教授，剛獲得美國國科會 (NSF) 五年三百萬美金的支持，為美國四個環境分子科學中心之一，其分析化學的能力，令人印

象深刻，他們更藉此能力，獲得許多重大的發現，譬如他們發現了 humic acid 在自然復育所扮的角色。

接著，我們拜訪環境工程系的 Prof. Harold Walker，他們的研究重點在於水質淨化，Ohio 為重要的煤礦產地，但其煤礦含硫量極高，同時也含有砷、汞等重金屬，這使地面、地下水含硫、含金屬量高。她們有很好的儀器作金屬離子偵測(AA 及 IPA),同時也探討如何以凝聚沉降技術純化水質。

中午，我們與化工系的 Prof. Jacques，Prof. Bhavuk Bakshi 一齊用餐，Prof. Zakin 提及日本如何節約能源，如何以循環水系統作建築物的暖化與冷卻似乎是大樓節約冷暖氣耗能的良好方法。

下午 Prof. Bakshi 介紹了如何用熱力學概念作為 Ecological、Industrial 及 Economical 系統整體評估的工具，現在生態評估、工業評估、及經濟評估的方式不同，因此難以作這三者相互影響的評估更無法提供不同程序對此三者之整體影響指標。他提出以 Energy 作為整體評估之度量基準，觀念新穎、前瞻，觀點具全面性。對 NSF 給與創新性研究的支持，也有極深刻的印象。(參見附錄二)

最後，我們與 Prof. Lianf-Shih Fan 的 Post doc.: Dr. Himanshu Gupta 會談，瞭解 Prof. Fan 這十年在清靜製程上的努力。他們發展了許多新的程序幫助減少燃燒煤炭時所造成的污染，也發展了方法以減少 CO₂ 的釋放，對如何使用化工技術進行清淨製程做了良好示範。

3.參訪心得

綠色製程技術主要的精神為：在製造之前與製造過程中，積極將減少資源耗費與降低廢棄物之排放列入主要考慮。所有有助於減少資源損耗，降低廢棄物排放，以及加速物質重複使用的技術與方法，都屬於綠色製程技術。但製程設計與製造技術是否真正符合綠色製程技術的精神，常常需要專業的評判。不僅需要作該技術在整體製程的評估，更要作區域生態與整體資源的評估，此評估，需要對物料進出、

能源進出詳細而整體的分析，也要對所使用的物料、能源與伴隨排放物對生態的影響，作詳細完整的分析，因此是極度需要化學、生物、工程與系統整合的技術。

(三)聖母大學化工系

1. 背景介紹：

聖母大學為天主教教會創立的私立大學。校園不大，但優雅如美國一般的大學城學校。該校工學院有電機工程，計算機工程，機械航太工程，土木地理系及化學工程系共五個系所，其中的化工系僅為中型大小，共有十五位教員，其主要的研究領域可概分為七項，其研究領域及相關之研究人員分述如下：

- (1)生化工程 - Agnes Ostafin 及 Andre Palmer 助理教授
- (2)催化及反應工程 - Hsueh-Chia Chang、 Arvind Varma 及 Eduardo E. Wolf 教授
- (3)複雜的流體及流動 - Hsueh-Chia Chang、 David T. Leighton、 Mark J. McCready 教授及 Davide A. Hill 副教授
- (4)清淨製程 - Joan F. Brennecke、 Mark J. McCready、 Roger A. Schmitz 及 Mark A. Stadtherr 教授
- (5)分子熱力學及統計力學 - Joan F. Brennecke 、 William C. Strieder 教授及 Edward J. Maginn 副教授
- (6)程序系統工程 - Jeffrey C. Kantor 副教授及 Mark A. Stadtherr 教授
- (7)科學及工程用之尖端材料 - Paul J. McGinn、 Albert E. Miller、 Arvind Varma 教授及 Davide A. Hill 和 Edward J. Maginn 副教授

2. 訪問經過

我們訪問自早上 10:30 開始至下午 4:40 結束，除化工系的教授外，我們亦與工學院院長，副校長見面暢談各半小時。Notre Dame 大學位在以農業為主的印第安那州。教授的研究與地區工業的關係就不如 Ohio State 大學密切，活躍，但對污染防治及綠色生產極為重視。教授們從與綠色生產關聯的研究主題開始影響研究生的觀念，進而在大學部的程序課程內容包含此方面的問題，讓學生思考污染防治與綠色生產。Brennecke 與 Stadtherr 教授負責四年級的程序設計，他們採

用 Allen 及 Shonnard 的新書(“Green Engineering : Environmentally Conscious Design of Chemical Processes” by David T. Allen and David R. Shonnard , Prentice Hall PTR , 2001)是目前考慮綠色生產最好及唯一的教科書。此教科書除化工製程的考慮外，還包含環保法規，經濟成本，生命週期等不同的方向看綠色生產的影響。此教科書的大綱具有參考價值，請參見附錄三。化工系在大學部開有環境相關的課程(1)讓學生了解產生污染物後的實際操作成本，如污染物的處理成本，亦即避免違反地區法規所需處理成本(2)讓學生了解製程降低污染的方法與措施(3)讓學生有機會利用新的無污染技術。這些觀念均包括於程序設計課程中。該系教授所強調的是如何利用對環境影響最低的化工新技術於製程中。學生的設計目前分別著重於分離程序中溶劑的改變，生產化學品過程中避免有毒中間體產生的製程，以及廢水處理和新技術發展。例如：

1.利用對環保極有利的超臨界二氧化碳萃取技術

- (1)超臨界二氧化碳萃取生薑中的生薑油(ginger oleoresin)
- (2)超臨界二氧化碳去除咖啡因
- (3)超臨界二氧化碳萃取大豆油
- (4)超臨界二氧化碳去除廢水中的酚
- (5)超臨界二氧化碳濃縮酒精
- (6)利用二氧化碳製造 dimethyl formamide

2.生產非破壞臭氧層的 R-134a 冷凍劑

3.生產 p-Nitroaniline 的新製程

4.廢水的清潔程序

- (1)超臨界 H₂O 氧化以淨化受酸污染之廢水
- (2)低溫觸媒氧化以淨化受酸污染之廢水
- (3)微電子產業廢水純化
- (4)受 VOC 污染的地下水淨化

5.不同反應步驟製造 Dimethyl Carbonate

6.回收 Polyethylene Terephthalate 設備的設計

該校工學院將投資 5 仟萬美金成立環境研究所 (Institute of Environment Research)領域包含化工系，土木地理系，機械航太系，

計算機系及電機系，社會系等。此外此環境研究所著眼於世界觀的環保問題，非僅關心印第安那州本土的環境保護問題。

以下為該系教授進行與環保相關的研究：

.超臨界 CO₂ 的應用

超臨界流體的應用研究已進行有二十年之久，因此此方向的研究並無特殊之處。目前 Brennecke 與 Stadherr 教授進行大豆油的萃取研究，目前距商業化甚遠，但若能有所突破則此新程序的貢獻極大。因目前大豆油的萃取利用極易燃的己烷而已商業化。其次利用超臨界 CO₂ 去咖啡因的關鍵操作，在於高溫的 CO₂ 並不需要減壓而回收繼續使用。此對能源有效使用，減低污染甚具效益。但此程序在國內無利用機會因國內不生產咖啡，超臨界流體運用，國內在此方面的研究不論在實驗，理論探討都已有基礎，化工所甚至運用於染色布料，對環保的貢獻更大。

.離子溶液(ionic solution)的應用

離子溶液為一種在常溫下為液體，具極低蒸汽壓的有機鹽，可溶於極性與非極性化合物。由於低蒸汽壓，因此既使在高溫 400 時此化合物仍然為液體。離子溶液的分子可以依運用時所需的性質再改變功能基合成而成。離子溶液的運用甚廣，但由於離子溶液的合成過程中，必須隔絕空氣，條件嚴格，因此離子溶液的成品價格高昂，而影響此方向的研究進展。離子溶液的運用包括：

(1)作為氫化，異構化，雙異構化，烷化反應等中間介質

離子溶液對反應速率，選擇性都優於傳統溶劑。由於離子溶液的低蒸汽壓，因此很容易與其他成份分離。一些氣體如：H₂，O₂，CO，C₂H₄ 在離子溶液的溶解度遠高於一般極性或非極性的有機溶劑。換言之，上述氣體在離子溶度的亨利常數遠大於在醇及己烷。因此上述氣體的反應速率在低壓情況下仍可較傳統的氣液反應較高。

(2)氣體分離

氣體在離子溶液的溶解度極大，如 CO₂ 在 40，50 bar 壓力下，在 [bmim][PF₆]₂ 的溶解度為 0.5 莫耳分率，而體積只增加 10%，此外溶解度不因改變離子溶液的陽離子，陰離子或功能基而改變，

此一特性確可運用於氣體混合物的分離，此特性遠比用傳統的液支薄膜(liquid supported membrane)分離優越，一般此種薄膜易因液體流失而損壞。

(3)液液分離

不同的化合物在不同的離子溶液中有不同的溶解度，利用此特性可以分離液相混合物。而且離子溶液的分子結構可以依需要而合成，因此利用離子溶液分離液相溶液應與分離氣體混合物相同值得探討。

(4)作為溶劑

許多極性及非極性化合物於離子溶液的溶解度極大，例如室溫下 naphthalene 在 [bmim][PF₆] 的溶解度約 30 mole%，因此以離子溶液取代傳統製程中有毒，易揮發的溶劑是清潔生產的一大貢獻。

(5)作為電解質 / 燃料電池原料

離子溶液具大電化學，高導電度，大溫度操作範圍，低介電常數，低揮發度及非燃性，作為電池的材料值得探討。

(6)作為潤滑劑

離子溶液易附著於金屬，高分子及無機物表面。加上離子溶液的熱穩定性及低蒸汽壓（高沸點）甚適合於作為高溫低壓條件下的潤滑劑。

(7)作為熱交換器流體

熱交換器流體的性質為熱穩定性高及大液相溫度範圍，而離子溶液的性質正適合作為熱交換器流體

觸媒轉換器的設計

汽車的觸媒轉換器在汽車剛開始啟動時轉換器溫度低，無法產生作用，此時排出氣體污染嚴重，為消除此問題，從理論模擬轉化器的動態變化，尤其分析汽車剛啟動時的狀況。此研究計畫重新設計汽車排放系統，不論車子的狀態如何，均能使汽車轉換器充分發揮其效果。

生態系統的模擬

R.A.Schmitz 教授利用計算機模擬地球的生態系統，結合生態與工程。一方面利用數學模式與計算機模擬，可以研究生態系統的動

態變化及地球生物化學週期。而另一方面，工程與地球科學家可以模擬地球的動態變化，以及人為的程序所釋放出的物質與能量如何影響環境。

次微孔隙粉末

Edward J. Maginn 教授正進行合成孔隙大小約 2~50 nm 的微孔粉末 (mesoporous powder)，此種沸石類粉未能自撐 (self supporting) 不需接合劑 (binder) 進而結構成填充床 (packed bed)，對重金屬有極高的吸附能力，對去除污染的土壤中的重金屬是極佳的吸附介質。

上述的研究都是化工系的教授們以化工的觀點解決環保的問題。在 Notre Dame 的訪問中，深深覺得，認為解決環保的問題是化學工程師的責任與工作。因為環保問題理論上還是化工的輸送，反應工程，熱力的範圍。

3. 參訪心得：

與 Carnegie Mellon 及 Ohio state 化工系教授討論時，可以感覺他們的研究題目甚富想像力，天馬行空，有些問題看起來不是很實際，卻是值得考慮的問題，但 Notre Dame 的教授們研究比較保守，有些題目都已在文獻上討論很多，如超臨界流體的運用，離子溶液的運用。然而 Notre Dame 化工系的研究均可實際應用於環境保護或綠色生產上，此為 Notre Dame 的一大特色。

此行可觀察出環境保護或綠色生產的研究都是以化學工程著眼，化工系的教授們為主，此與台灣的環境問題都由環工系所把握為主的情況有極大的差異。

五、結語與建議

此次參訪更加深成立『綠色設計及製造中心』的規劃，我們可利用發展中的清淨製程相關技術與產業界進行技術交流，利用專題研究計劃的進行，提供工業界設計方針與製造技術的支援，其合作的主題如下：

1. 綠色設計相關的程序系統工程：新一代的程序系統工程，除了需具備整廠設計控制觀念外，還需著眼於整體企業、完整生態，本子項目的在提昇國內工業界所需化工人才之綠色設計、程序控制與系統整合能力，進而發展安全、可靠、清淨而無公害的製程技術，以降低製造成本，提高生產物品質。其產學合作重點包括：

設計相關領域：反應系統、蒸餾系統、反應性蒸餾、共沸蒸餾、整廠製程、電子材料製程與再生能源製程之開發與改善，重點將以程序與產品生命周期分析來降低對環境的衝擊。

控制相關領域：非線性控制、PID 控制調諧、韌性控制、多變數控制、程序監控與診斷、專家系統及供給鏈管理(SCM)等，將著重綠色製程的可操作度。

2. 綠色設計相關的基本製程技術：除了已知製程的設計與操作上的改進外，本中心更著眼於新製程的開發。這包括：新材料的合成、新反應機構的找尋、新分離技術的開發及相關的工程技術。配合化工學門的重點，本子項將著重於：

基礎製程：省能材料合成、高性能觸媒、高效率電池的技術開發及如薄膜等低耗能分離程序之開發。

工程技術：熱交換網路技術的開發、熱回收之新技術開發等。

3. 污染防治：除了著重製程減廢外，污染防治仍將是重點，不同於傳統的設計，中心之重點應加強質量交換網路的概念，從設計、操作、

及控制等方面著手，以降低營運成本。研究重點方向包括：

工業廢水高級處理技術之開發；

環境管理與製程減廢；

空氣污染控制技術；

工業廢棄物之處理與處置。

六、附錄

(一) A. 卡內基美隆大學化工系 ICES 簡介



Institute for Complex Engineered Systems

Cristina H. Amon
Director

Advanced Infrastructure Systems
Jim Garrett
jim.garrett@ices.cmu.edu

Computational Analysis of Social and Organizational Systems (CASOS)
Kathleen Carley
kathleen.carley@ices.cmu.edu

Education
Art Westerberg
art.westerberg@ices.cmu.edu

Embedded & Reliable Information Systems (ERIS)
Phil Koopman
phil.koopman@ices.cmu.edu

Engineering Design Research Center (EDRC)
Susan Finger
susan.finger@ices.cmu.edu

Interaction Design Studio
Francine Gemperle
francine.gemperle@ices.cmu.edu

Micro Electro-Mechanical Systems (MEMS)
Gary Fedder
gary.fedder@ices.cmu.edu

Thermal Management & Electronic Cooling
Jayathi Murthy
jayathi.murthy@ices.cmu.edu

Tissue Engineering & Artificial Organs
Lee E. Weiss
lee.weiss@ices.cmu.edu

Institute for Complex Engineered Systems
Carnegie Mellon University
College of Engineering
1201 Hamburg Hall
Pittsburgh, PA 15213-3890

ph: 412.268.3372
fax: 412.268.5229
www.ices.cmu.edu

Carnegie Mellon

Industrial Affiliates Program and Benefits

AFFILIATE

Annual fee: \$25,000

- Papers and Technical Reports
- Invitation to Annual Symposium
- Access to Undergraduate and Graduate Students in the Institute
- Small Company Provision (for gross sales < \$50M) – \$10,000

MEMBER

Annual fee: \$60,000

- Affiliate Membership Benefits
- Additional Benefits:
 - Industrial Board membership
 - Quick turnaround demo/project or scoping study using company data
- Small Company Provision (for gross sales < \$50M) – \$30,000

PARTNER

Annual fee: \$100,000-\$150,000

- Membership Benefits
- Additional Benefits:
 - Collaborate on a project of the Partner's interest
 - Possible student internship at company
 - Software for internal use on one project of interest

STRATEGIC PARTNER

Annual fee: \$200,000-\$300,000

- Partnership Benefits
- Additional Benefits:
 - Placement of a research scientist or engineer at ICES
 - Co-advising of graduate students
 - Preferred partnering on joint proposals to Federal Agencies
 - Joint project course with company involvement



(一) B. 卡內基美隆大學化工系 CAPD 簡介

The Center for Advanced Process Decision-making (CAPD) is a unique research group that deals with the development of methodologies and computer tools for process industries.

The CAPD consortium currently lists over 20 members from the chemical and petroleum industries as well as a number of hardware and software companies. Research work is directed by Professors Biegler, Grossmann, Huan, Powers, Westerberg, and Ydstie and is carried out by over 30 graduate students and researchers from the Department of Chemical Engineering. The main areas of research include modeling and simulation, process synthesis, process optimization, process control, scheduling and planning, supply chain management, and information modeling.

CAPD Current Members

Air Products and Chemicals
ALCOA
Aristech Chemical Corporation
Aspen Technology
Bayer
BPA/Amoco
Dash Optimization
Dow Chemical Company
DuPont Corporation
Eastman Chemical Company
Elf Total
ELKEM
Exxon/Mobil Company
GAMS Development Corporation
Honeywell Inc.
Kraft Foods, Inc.
Mitsubishi Chemical Corporation
Neste Engineering Oy
Simulation Sciences, Inc.

The Chemical Engineering Department

Doherty Hall
Carnegie Mellon University
Pittsburgh, PA 15213
(412) 268-6344
FAX: (412) 268-7239
lr23@andrew.cmu.edu

Center for Advanced Process Decision-making



CAPD
CENTER

Carnegie Mellon

Department of Chemical Engineering

www.cheme.cmu.edu/research/capd

Annual Review

The consortium holds an Annual Review for all members early each spring. Held over a two-day period, this meeting includes reviews of all CAPD projects as well as general discussions between graduate students and these members of industry.

Publications

Every semester the CAPD issues a newsletter providing a progress report on each of the projects. Included with the newsletter are copies of the most recent research publications.

Some Specific Research Topics:

- Synthesis of reactor networks, complex azeotropic/reactive/separation and energy systems
- Structural flowsheet optimization and retrofit design
- Multiperiod design and planning of batch and continuous process systems
- Planning and optimization at oil field facilities
- Process scheduling, supply chain management, new product development
- Thermodynamics-based process control
- Process verification
- Optimization strategies for process control and parameter estimation
- Large-scale nonlinear programming
- Optimization of differential-algebraic systems
- Strategies for mixed-integer programming

- Logic based optimization and disjunctive programming for process synthesis and scheduling
- Advanced environments for the rapid creation, debugging, and solution of large, complex equation-based models
- Environment for capturing, structuring, and sharing of information to support team based engineering design
- Adaptive control and on-line parameter estimation
- Modeling simulation and control of distributed systems
- Verification of control system software and human operating procedures

CAPD Short Course

The consortium also offers a short course in June, with members receiving a 25% discount registration fee. Individual meetings are also encouraged with industrial representatives to define new projects and discuss current work.

CAPD Software

The consortium also makes software available to its members, although some programs require a license if it uses another commercial package. Some of these programs include:

- **rSQP** Successive quadratic programming for nonlinear optimization
- **DICOPT++** General purpose code for mixed-integer nonlinear optimization

- **SYNHEAT, STEAM** Synthesis programs for heat exchanger networks, utility systems.
- **STBS, BATCHSPC, PLANNER** Programs for scheduling and planning
- **LOGMIP** Code for disjunctive programming
- **GAMS** PC based interfaces for process synthesis, planning and scheduling
- **ASCEND** Equation based modeling system
- **n-dim** Information management systems

Membership

The annual fee for membership in the consortium is \$16,500. These are unrestricted funds for research and to primarily support graduate students (each student's tuition and stipend exceeds \$50,000 per year)

For more information, contact Ms. Laura Shaheen at (412-268-6344), e-mail: lr23@andrew.cmu.edu, or contact us via wwwcheme.cmu.edu/research/capd



(二) Bakshi 教授有關環境自覺程序系統工程之簡報資料

**A Thermodynamic Framework
for Ecologically Conscious
Process Systems Engineering**

Bhavik R. Bakshi

Department of Chemical Engineering
Ohio State University
Columbus, OH 43210

Motivation

- Chemical Engineering has played an important role in human prosperity
 - Energy technology, Medicinal products, New materials
- Significant impact of our activities on the environment
 - Pollution, Ozone depletion, Climate change, Biodiversity loss
- Need for sustainable human activities (WCED, 1987)
 - "... meets the needs of the present without compromising the ability of future generations to meet their own needs."
- For long-term competitive advantage industry must consider ecological, economic, and social aspects (Holiday, 1994; DeSimone and DePaoli, 1997)

Traditional Approach

- Considers environment as secondary to more important economic activity
 - Emphasis on reducing level and immediate risk
 - Focus on remediation and compliance
 - Narrow focus on process scale
- Money is an incomplete measure of environmental inputs and impact
- May solve only part of the problem or shift impact to another domain
- Need "systems" view to go beyond scale of the process

**Life Cycle Management
Approach**

- Aims to consider environmental, economic and social aspects throughout life cycle
- Included techniques for:
 - Life Cycle Assessment (LCA) of products
 - Design for the environment
 - Environmental accounting
- Essential for implementing industrial ecology
- Used for various PSE tasks (Kawachi, 1989; Pantazopoulos, 1996; Gosselin et al., 1999)
- Significant advance over traditional methods

**Shortcomings of Existing
Methods**

- Lack of common framework for the analysis of industrial, ecological, and economic systems
- Ecological methods ignore impact of emissions
- Engineering methods ignore contribution of ecological products and services
 - Such as wind, river flow, rain, photosynthesis, pollination, biodegradation
 - Nature's services are estimated to be worth about 1.3 times global gross national product (Costanza et al., 1997)
 - Can introduce significant error in LCA results
- Widespread deterioration of ecosystem condition and services

Consequences of Shortcomings

- Deterioration of ecological services
 - 35% decline in ecosystems, with 90% increase in human pressure in last 50 years (WWF, 2000)
 - 50% of world's wetlands lost in last century (WWF, 2000)
 - 88% of coral reefs impaired by human activity
 - 80% grasslands suffering from soil degradation
- Chemical engineers have a special responsibility and opportunity since
 - Chemical industry dominates in generating hazardous waste
 - More than 75,000 chemicals developed in last 50 years
 - Generation of industrial waste in the U.S. is more than 100 billion (kilobyte) tons and tons (BASF, 1997)
 - Harmful effects of DDT, DDE, etc.

Objectives

- Develop rigorous framework for incorporating ecological and economic considerations in industrial tasks
- Exploit synergy between methods in
 - Systems Ecology
 - Process Systems Engineering
 - Life Cycle Assessment
- Apply framework to solve PSE tasks
 - Life cycle assessment of products
 - Chemical process design
 - Process operation, etc.

Outline

- Introduction to Systems Ecology
 - Characteristics of ecological systems
 - Energy flow diagrams
 - Emergy, Exergy, Transformity
- Thermodynamic framework for the analysis of industrial and ecological systems
- Analysis of economic and ecological inputs
- Thermodynamic analysis of environmental impact
- Emergy-based life cycle assessment of products
- Summary and future work

Characteristics of Ecological Systems

- Development and growth are limited by the availability of resources and the ability to exploit them
- All resources and services are transformed and stored solar energy
- Ecosystems are networks of energy flow
- Historical perspective
 - "life is a struggle for the ability to perform work" (Saltzman, 1945)
 - systems process that develop designs that maximize the flow of useful energy (Lofka, 1922)
 - "continually making orderliness from its environment" (Schulzinger, 1967)

Energy Flow Diagrams

- Used extensively for representing, analyzing, and modeling ecosystems (coal, iron, steel, etc., steel)
- Energy flow in food chain

- Available energy per unit of solar energy decreases
- Ability to do work and energy concentration increase
- Analysis requires concepts of **emergy** and **exergy**

Emergy, Exergy, Transformity

- Available Energy or **exergy** is the energy that can be converted to useful work
- Embedded Emergy** or **emergy** is the total energy needed directly or indirectly to make a product or service
- Emergy = Transformity X Exergy

$\frac{\text{Joules}}{\text{Joule}}$ (Transformity)
Joules (Exergy)
Joules (Emergy)

Properties of Emergy and Exergy

- Emergy and exergy are complementary properties

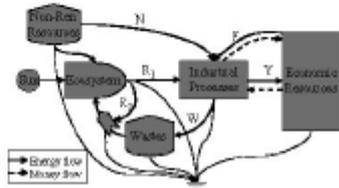
Emergy	Exergy
Measure of energy past	Measure of energy future
Inputs from environment	Output to environment
Path dependent	State dependent

- Emergy is the cumulative exergy consumed starting from solar energy
- Transformity is inversely proportional to efficiency
- Higher transformity indicates greater ability to do work, that is, higher quality of energy

Analysis of Industrial and Ecological Systems

- Industrial processes transform ecological products and services into economic products and services
- Both systems are networks of energy flow and satisfy same laws of nature
- Emergy is a measure of ecological involvement
 - Can be used as a common currency to measure ecological cost
 - Money is an incomplete measure
- Permits joint analysis of ecological and economic aspects of industrial systems

Energy Flow Diagram of IE Processes



- Energy and exergy flows can be determined from material and energy balances

Flow from Economic Inputs

- Economic inputs have monetary value
 - Labor, fuel, equipment, etc.
- May be determined from
 - Life cycle inventory data
 - Material input-output tables
- May be approximated from economic data
 - Cost of inputs
 - Economic input-output tables
- Emergy = economic cost \times $\frac{\text{total emergy input}}{\text{gross economic product}}$

Flow from Ecological Inputs

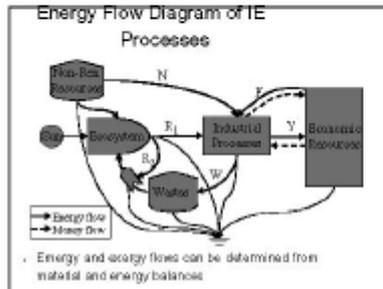
- Ecological inputs can be renewable or nonrenewable
 - Sunlight, Rain, Wind, Fertile soil, Biodegradation, etc.
- Ecological services and products are needed
 - As inputs for economic activity used
 - For detoxifying and absorbing emissions
- Emergy in ecological inputs can be determined from their transformity
 - Tabulated by ecologists (Odum, 1980)
 - Relatively constant due to evolutionary processes
 - Solar transformity = 1 sej/J, wind = 1.0E+5, crude = 5.4E+4, Limestone = 1.0 E+6 sej/J

Thermodynamic Analysis of Impact

- Response of self-organized systems to stress
 - Stressed systems lose energy, move closer to equilibrium
 - Disturbance introduces energy that causes reduction in ecosystem energy (Odum, 1980)
- Exergy loss due to perturbation provides holistic measure of impact
- Combine with Life Cycle Impact Assessment methods
 - Need to convert LCA output to exergy loss
 - Require appropriate LCA methods

Exergy Loss via Life Cycle Impact Assessment

- Eco-Indicator 99 assesses damage to (Kloppsch and Spriensma 2000)
 - Human health measured by DALY
 - Ecosystem quality measured by PAF and PDF
 - Resources
- Disability Adjusted Life Years (DALY) combines years of life lost and years lived disabled (WHO, 1994)
- Potentially Affected Fraction (PAF) of species is determined by ecological models
- Need to convert impact in each category to exergy loss



Exergy Loss Due to Impact

- Determine exergy loss of impact on human health and ecosystem quality
- Combine DALY and PAF with exergy of affected species
- Exergy of living organisms may be computed by combining
 - Traditional contributions (chemical, physical exergy)
 - Contribution from genetic information content (degrees of freedom)
- Approximate exergy per human = $43 \cdot 10^{18}$ Joules

Performance Metrics

- Exergy gain for economy (Net exergy) = $Y - F$
 - Net exergy must be positive for industrial processes to be beneficial to the economy
- Exergy ROI for economy (Exergy Yield Ratio) = Y/F
 - Analogous to return on investment
 - Compares resource consumption with value creation
- Environmental loading ratio = $(F+N+R_2)/R_1$
- Sustainability metric = $E^*/R_1/CLR$
- Useful for analysis and comparison of ecological and economic aspects (Odum, 1983; Brown and Ugelstad, 1987)

LCA of Soy Bean Growth

- LCA focuses on abiotic and energy depletion and impact of emissions
- Classification and characterization of emissions per ton of soy bean oil (Heungs et al., 1996)

- Global Warming Potential	43.5 kg
- Human Toxicity	15.0 kg
- Photochemical Oxidant Creation	0.02 kg
- Acidification	0.31 kg
- Nutrient	41.6 kg
- Impacts are combined in valuation step

emLCA of Soy Bean Growth

- Energy-based LCA considers all the inputs
 - Renewable resources (R_1) - sun, air, soil
 - Non-renewable resources (N) - loss of fossil
 - Economic resources (F) - labor, fuel, services
 - Absorption of Waste (R_2) - LCA categories, wind
- Selected energy flows for emLCA (per ton of soy oil)

R_1 Sunlight	$1.8E+14$	Rain	$6.6E+14$
M Soil erosion	$1.3E+18$		
F Labor	$4.9E+14$	Fertilizers	$1.1E+18$
R_2 Human health	$7.1E+17$		
- Ecological and economic inputs are comparable - neither can be ignored

Ecologically Conscious Process Design

- Evaluate both, economic and thermodynamic yield of selected design
- Pose selected sustainability index as constraint
- May use multiobjective optimization to find Pareto optimal surface
- Select "optimum" based on valuation of economic and ecological aspects
- Can be used to determine modifications to make process more sustainable

Summary

- Contribution of nature's services to industrial activity MUST be taken into account
- Thermodynamics can provide systematic framework for analysis of industrial and ecological systems
 - Address both value creation and resource consumption
- Emergy analysis provides
 - Measure of ecological cost
 - Common currency for all systems
- Life cycle inventory can provide emergy of economic inputs
- Systems ecology provides emergy of ecological inputs
- LCA provides information about impact of emissions

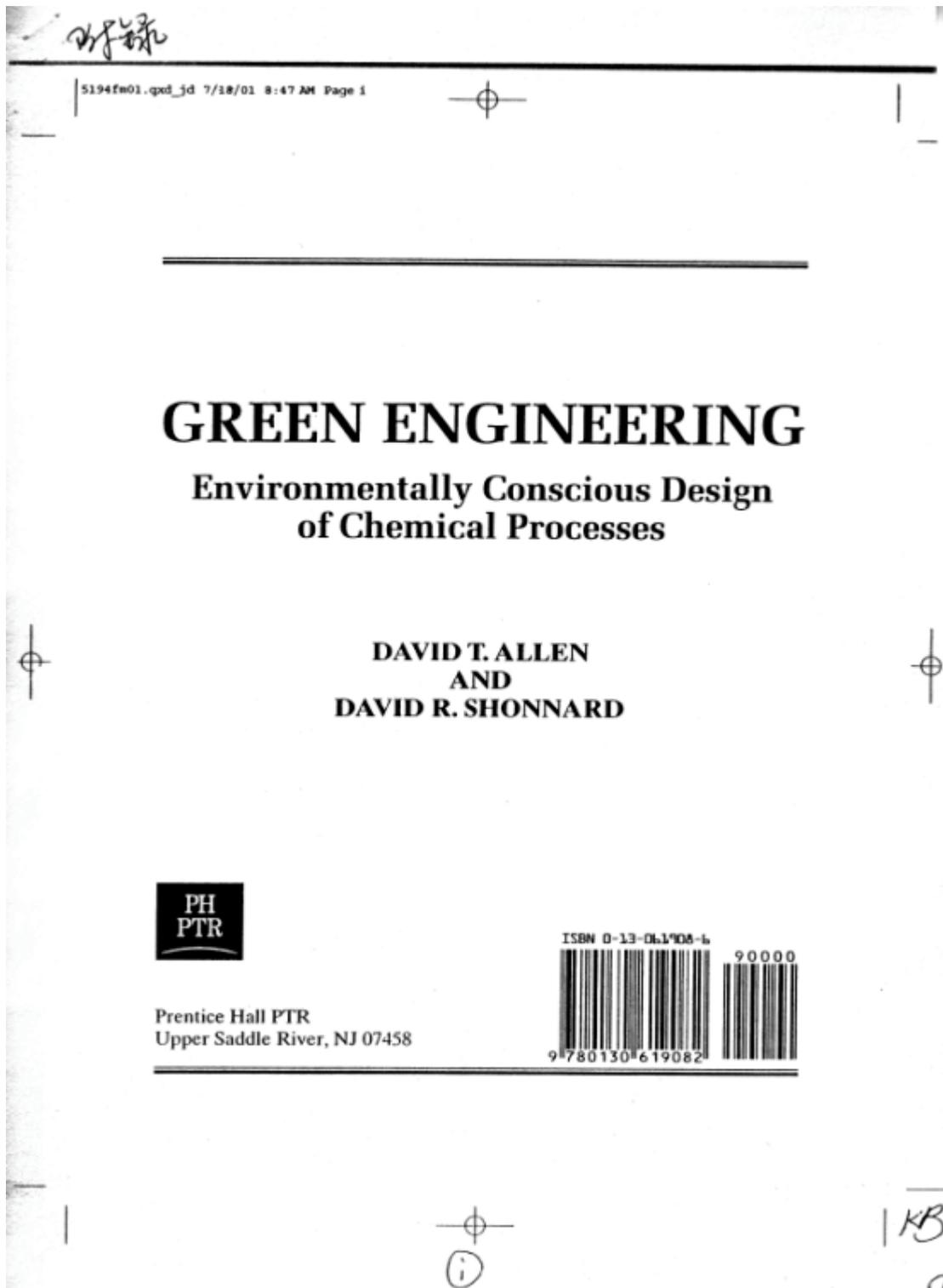
Future Work

- Many challenges to make framework practical
 - Life cycle inventory data with ecological inputs
 - Transformation of ecological and economic products and services
 - Thermodynamic analysis of impact
- Many potential applications
 - Sustainability engineering
 - Process design and retrofit
 - Product assessment and design
 - Green chemistry
- Requires multidisciplinary collaboration!

Acknowledgments

- NSF/EPA Program on Technology for a Sustainable Environment, (DCE-9603354)
- Mr. Jorge Hsu
- Mr. Nandan Uddwe
- Dr. Joseph Fiksel and the Life Cycle Management group at Battelle

(三) Green Engineering : Environmentally Conscious Design of Chemical Processes 教科書之課程大綱





Library of Congress Cataloging-in-Publication Data

Allen, David T.
Green engineering : environmentally conscious design of chemical processes / by David Allen and David Shonnard.
p. cm.
Includes bibliographical references and index.
ISBN 0-13-061908-6
1. Environmental chemistry—Industrial applications. 2. Environmental management. I. Shonnard, David. II. Title.

TP155.Z.E58 A54 2002
660—dc21

2001034380

Editorial/Production Supervision: *Kerry Reardon*
Production Coordinator: *Anne R. Garcia*
Acquisitions Editor: *Bernard Goodwin*
US EPA Editor: *Sharon L. Austin*
Marketing Manager: *Dan DePasquale*
Manufacturing Manager: *Alexis R. Heydt-Long*
Cover Design Director: *Jerry Votta*
Cover Design: *Anthony Gemmellaro*
Cover Photo: ©2002 *www.ArtToday.com*
Art Director: *Gail Cocker-Bogusz*
Editorial Assistant: *Michelle Vincenti*
Composition: *Pine Tree Composition*



© 2002 Prentice Hall PTR
Prentice-Hall, Inc.
Upper Saddle River, NJ 07458

Prentice Hall books are widely used by corporations and government agencies for training, marketing, and resale.

The publisher offers discounts on this book when ordered in bulk quantities. For more information, contact Corporate Sales Department, phone: 800-382-3419; fax: 201-236-7141; e-mail: corpsales@prenhall.com or write: Prentice Hall PTR, Corporate Sales Department, One Lake Street, Upper Saddle River, NJ 07458

All rights reserved. No part of this book may be reproduced, in any form or by any means, without permission in writing from the publisher.

All products or services mentioned in this book are the trademarks or service marks of their respective companies or organizations.

Printed in the United States of America on 30% post-consumer recycled fiber.

Printed in the United States of America
10 9 8 7 6 5 4 3 2 1

ISBN 0-13-061908-6

Pearson Education LTD.
Pearson Education Australia PTY, Limited
Pearson Education Singapore, Pte. Ltd.
Pearson Education North Asia Ltd.
Pearson Education Canada, Ltd.
Pearson Educacion de Mexico, S.A. de C.V.
Pearson Education—Japan
Pearson Education Malaysia Pte. Ltd.
Pearson Education, Upper Saddle River, New Jersey



AB

Contents

PREFACE	xiii
ABOUT THE AUTHORS	xv
ACKNOWLEDGMENTS	xix
PART I A CHEMICAL ENGINEER'S GUIDE TO ENVIRONMENTAL ISSUES AND REGULATIONS	1
I AN INTRODUCTION TO ENVIRONMENTAL ISSUES	3
1.1 Introduction, 3	
1.2 The Role of Chemical Processes and Chemical Products, 4	
1.3 An Overview of Major Environmental Issues, 6	
1.4 Global Environmental Issues, 7	
1.4.1 Global Energy Issues, 7	
1.4.2 Global Warming, 9	
1.4.3 Ozone Depletion in the Stratosphere, 10	
1.5 Air Quality Issues, 14	
1.5.1 Criteria Air Pollutants, 15	
1.5.1.1 NO _x , Hydrocarbons, and VOC's—Ground-Level Ozone, 17	
1.5.1.2 Carbon Monoxide, 17	
1.5.1.3 Lead, 19	
1.5.1.4 Particulate Matter, 19	
1.5.1.5 SO ₂ , NO _x , and Acid Deposition, 20	
1.5.2 Air Toxics, 21	
1.6 Water Quality Issues, 22	
1.7 Ecology, 23	

1.8	Natural Resources,	24
1.9	Waste Flows in the United States,	24
	Summary,	28
	References,	29
	Problems,	30

2 RISK CONCEPTS 35

2.1	Introduction,	35
2.2	Description of Risk,	36
2.3	Value of Risk Assessment in the Engineering Profession,	39
2.4	Risk-Based Environmental Law,	41
2.5	General Overview of Risk Assessment Concepts,	42
2.6	Hazard Assessment,	44
	2.6.1 <i>Cancer and Other Toxic Effects,</i>	45
	2.6.2 <i>Hazard Assessment for Cancer,</i>	46
	2.6.3 <i>Hazard Assessment for Non-Cancer Endpoints,</i>	48
	2.6.4 <i>Structure Activity Relationships (SAR),</i>	50
	2.6.5 <i>Readily Available Hazard References,</i>	50
2.7	Dose-Response,	52
2.8	Exposure Assessment,	54
2.9	Risk Characterization,	57
	2.9.1 <i>Risk Characterization of Cancer Endpoints,</i>	57
	2.9.2 <i>Risk Characterization of Non-Cancer Endpoints,</i>	57
	2.9.3 <i>Adding Risks,</i>	58
	Summary,	58
	References,	58
	Problems,	60

3 ENVIRONMENTAL LAW AND REGULATIONS: FROM END-OF-PIPE TO POLLUTION PREVENTION 63

3.1	Introduction,	63
3.2	Nine Prominent Federal Environmental Statutes,	66
3.3	Evolution of Regulatory and Voluntary Programs: From End-of-Pipe to Pollution Prevention,	67
3.4	Pollution Prevention Concepts and Terminology,	70
	References,	76
	Problems,	77

Contents	vii
4 THE ROLES AND RESPONSIBILITIES OF CHEMICAL ENGINEERS	81
4.1 Introduction, 81	
4.2 Responsibilities for Chemical Process Safety, 82	
4.3 Responsibilities for Environmental Protection, 85	
4.4 Further Reading in Engineering Ethics, 87	
References, 87	
Problems, 88	
PART II EVALUATING AND IMPROVING ENVIRONMENTAL PERFORMANCE OF CHEMICAL PROCESSES	91
5 EVALUATING ENVIRONMENTAL FATE: APPROACHES BASED ON CHEMICAL STRUCTURE	93
5.1 Introduction, 93	
5.2 Chemical and Physical Property Estimation, 95	
5.2.1 Boiling Point and Melting Point, 97	
5.2.2 Vapor Pressure, 100	
5.2.3 Octanol-Water Partition Coefficient, 103	
5.2.4 Bioconcentration Factor, 108	
5.2.5 Water Solubility, 110	
5.2.6 Henry's Law Constant, 112	
5.2.7 Soil Sorption Coefficients, 115	
Summary, 118	
Questions for Discussion, 118	
5.3 Estimating Environmental Persistence, 118	
5.3.1 Estimating Atmospheric Lifetimes, 118	
5.3.2 Estimating Lifetimes in Aqueous Environments, 122	
5.3.3 Estimating Overall Biodegradability, 124	
Summary, 126	
Questions for Discussion, 126	
5.4 Estimating Ecosystem Risks, 126	
Questions for Discussion, 127	
5.5 Using Property Estimates to Estimate Environmental Fate and Exposure, 127	
Summary, 131	
Questions for Discussion, 131	
5.6 Classifying Environmental Risks Based on Chemical Structure, 131	
References, 133	
Problems, 135	



6	EVALUATING EXPOSURES	139
6.1	Introduction, 139	
6.2	Occupational Exposures: Recognition, Evaluation, and Control, 140	
6.2.1	<i>Characterization of the Workplace, 141</i>	
6.2.2	<i>Exposure Pathways, 143</i>	
6.2.3	<i>Monitoring Worker Exposure, 145</i>	
6.2.4	<i>Modeling Inhalation Exposures, 146</i>	
6.2.4.1	<i>The Mass Balance Model, 146</i>	
6.2.4.2	<i>Dispersion Models, 149</i>	
6.2.5	<i>Assessing Dermal Exposures, 151</i>	
	<i>Questions for Discussion, 156</i>	
6.3	Exposure Assessment for Chemicals in the Ambient Environment, 156	
6.3.1	<i>Exposure to Toxic Air Pollutants, 156</i>	
6.3.2	<i>Dermal Exposure to Chemicals in the Ambient Environment, 160</i>	
6.3.3	<i>Effect of Chemical Releases to Surface Waters on Aquatic Biota, 161</i>	
6.3.4	<i>Ground Water Contamination, 164</i>	
	<i>Questions for Discussion, 167</i>	
6.4	Designing Safer Chemicals, 167	
6.4.1	<i>Reducing Dose, 168</i>	
6.4.2	<i>Reducing Toxicity, 169</i>	
	References, 170	
	Problems, 172	
7	GREEN CHEMISTRY	177
7.1	Green Chemistry, 177	
7.2	Green Chemistry Methodologies, 178	
7.2.1	<i>Feedstocks, 178</i>	
7.2.2	<i>Solvents, 181</i>	
7.2.3	<i>Synthesis Pathways, 185</i>	
7.2.4	<i>Functional Group Approaches to Green Chemistry, 190</i>	
7.3	Quantitative/Optimization-Based Frameworks for the Design of Green Chemical Synthesis Pathways, 191	
7.4	Green Chemistry Expert System Case Studies, 195	
	Questions for Discussion, 196	
	References, 196	
	Problems, 198	
8	EVALUATING ENVIRONMENTAL PERFORMANCE DURING PROCESS SYNTHESIS	199
8.1	Introduction, 199	



MB

8.2	Tier 1 Environmental Performance Tools,	200
8.2.1	<i>Economic Criteria,</i>	201
8.2.2	<i>Environmental Criteria,</i>	202
8.2.3	<i>Threshold Limit Values (TLVs), Permissible Exposure Limits (PELs), and Recommended Exposure Limits (RELs),</i>	204
8.2.4	<i>Toxicity Weighting,</i>	207
8.2.5	<i>Evaluating Alternative Synthetic Pathways,</i>	209
	<i>Questions for Discussion,</i>	215
8.3	Tier 2 Environmental Performance Tools,	215
8.3.1	<i>Environmental Release Assessment,</i>	216
8.3.1.1	<i>Basics of Releases,</i>	216
8.3.1.2	<i>Release Assessment Components,</i>	216
8.3.1.3	<i>Process Analysis,</i>	217
8.3.2	<i>Release Quantification Methods,</i>	220
8.3.2.1	<i>Measured Release Data for the Chemical,</i>	220
8.3.2.2	<i>Release Data for a Surrogate Chemical,</i>	221
8.3.2.3	<i>Emissions Factors,</i>	221
8.3.2.4	<i>Emissions from Process Units and Fugitive Sources,</i>	222
8.3.2.5	<i>Losses of Residuals from Cleaning of Drums and Tanks,</i>	225
8.3.2.6	<i>Secondary Emissions from Utility Sources,</i>	228
8.3.3	<i>Modeled Release Estimates,</i>	231
8.3.3.1	<i>Loading Transport Containers,</i>	231
8.3.3.2	<i>Evaporative Losses from Static Liquid Pools,</i>	237
8.3.3.3	<i>Storage Tank Working and Breathing Losses,</i>	238
8.3.4	<i>Release Characterization and Documentation,</i>	239
8.3.5	<i>Assessing Environmental Performance,</i>	244
	<i>Questions for Discussion,</i>	246
8.4	Tier 3 Environmental Performance Tools,	246
	References,	246
	Problems,	248

9 UNIT OPERATIONS AND POLLUTION PREVENTION 251

9.1	Introduction,	251
9.2	Pollution Prevention in Material Selection for Unit Operations,	253
9.3	Pollution Prevention for Chemical Reactors,	257
9.3.1	<i>Material Use and Selection for Reactors,</i>	258
9.3.2	<i>Reaction Type and Reactor Choice,</i>	261
9.3.3	<i>Reactor Operation,</i>	268
9.4	Pollution Prevention for Separation Devices,	274
9.4.1	<i>Choice of Mass Separating Agent,</i>	274
9.4.2	<i>Process Design and Operation Heuristics for Separation Technologies,</i>	276

- 9.4.3 *Pollution Prevention Examples for Separations*, 280
- 9.4.4 *Separators with Reactors for Pollution Prevention*, 280
- 9.5 *Pollution Prevention Applications for Separative Reactors*, 283
- 9.6 *Pollution Prevention in Storage Tanks and Fugitive Sources*, 286
 - 9.6.1 *Storage Tank Pollution Prevention*, 286
 - 9.6.2 *Reducing Emissions from Fugitive Sources*, 289
- 9.7 *Pollution Prevention Assessment Integrated with HAZ-OP Analysis*, 294
- 9.8 *Integrating Risk Assessment with Process Design—A Case Study*, 296
- Questions for Discussion, 301
- References, 301
- Problems, 305

10 FLOWSHEET ANALYSIS FOR POLLUTION PREVENTION **309**

- 10.1 *Introduction*, 309
- 10.2 *Process Energy Integration*, 313
- 10.3 *Process Mass Integration*, 317
 - 10.3.1 *Source-Sink Mapping*, 317
 - 10.3.2 *Optimizing Strategies for Segregation, Mixing, and Recycle of Streams*, 327
 - 10.3.3 *Mass Exchange Network Synthesis*, 333
- 10.4 *Case Study of a Process Flowsheet*, 347
- Summary, 354
- References, 354
- Problems, 355

11 EVALUATING THE ENVIRONMENTAL PERFORMANCE OF A FLOWSHEET **361**

- 11.1 *Introduction*, 361
- 11.2 *Estimation of Environmental Fates of Emissions and Wastes*, 362
 - 11.2.1 *Fugacity and Fugacity Capacity*, 364
 - 11.2.2 *Intermedia Transport*, 367
 - 11.2.3 *Reaction Loss Processes*, 371
 - 11.2.4 *Balance Equations*, 372
- 11.3 *Tier 3 Metrics for Environmental Risk Evaluation of Process Designs*, 375
 - 11.3.1 *Global Warming*, 376
 - 11.3.2 *Ozone Depletion*, 378
 - 11.3.3 *Acid Rain*, 379
 - 11.3.4 *Smog Formation*, 379
 - 11.3.5 *Toxicity*, 386
- Summary, 390
- References, 392
- Problems, 394

Contents	xi
12 ENVIRONMENTAL COST ACCOUNTING	397
12.1 Introduction, 397	
12.2 Definitions, 398	
12.3 Magnitudes of Environmental Costs, 400	
12.4 A Framework for Evaluating Environmental Costs, 402	
12.5 Hidden Environmental Costs, 405	
12.6 Liability Costs, 407	
12.7 Internal Intangible Costs, 412	
12.8 External Intangible Costs, 413	
References, 414	
Problems, 415	
PART III MOVING BEYOND THE PLANT BOUNDARY	417
13 LIFE-CYCLE CONCEPTS, PRODUCT STEWARDSHIP, AND GREEN ENGINEERING	419
13.1 Introduction to Product Life Cycle Concepts, 419	
13.2 Life-Cycle Assessment, 421	
13.2.1 Definitions and Methodology, 422	
13.2.2 Life-Cycle Inventories, 425	
13.3 Life-Cycle Impact Assessments, 432	
13.3.1 Classification, 433	
13.3.2 Characterization, 433	
13.3.3 Valuation, 437	
13.3.4 Interpretation of Life-Cycle Data and Practical Limits to Life-Cycle Assessments, 440	
13.4 Streamlined Life-Cycle Assessments, 441	
13.4.1 Streamlined Data Gathering for Inventories and Characterization, 441	
13.4.2 Qualitative Techniques for Inventories and Characterization, 442	
13.4.3 Pitfalls, Advantages, and Guidance, 447	
13.5 Uses of Life-Cycle Studies, 448	
13.5.1 Product Comparison, 448	
13.5.2 Strategic Planning, 448	
13.5.3 Public Sector Uses, 448	
13.5.4 Product Design and Improvement, 450	
13.5.5 Process Design, 453	
Summary, 453	
Questions for Discussion, 455	
References, 455	
Problems, 457	