行政院所屬各機關因公出國人員出國報告書
（出國類別：國際會議）

出席空氣品質模式發展研討會

服務機關：行政院環境保護署
姓名職稱：林雍嵐技士
派赴國家：美國
出國期間：民國 105 年 10 月 23 日至 10 月 29 日
報告日期：民國 106 年 1 月 10 日

出國報告(出國類別：國際會議)

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摘要

職於 2016 年 10 月 24 至 26 日間前往美國北卡羅萊納州教堂山出席第 15 屆空氣品質模式發展研討會(The 15th Annual Community Modeling and Analysis System Conference)。本次研討會為期 3 日，議程涵蓋空氣品質模式發展、先進氣象模式近期改善與發展、高解析模式模擬應用、模式個案診斷分析、氣象場對空氣品質模式準確度之敏感度測試、全球與區域模式運用、氣候變遷與能源等議題，與會的環境部門代表及學術研究人員分別來自美國、加拿大、巴西、哥倫比亞、中國大陸、印度、法國、日本及臺灣等共計 13 個國家，各國代表及專家學者透過研討交流，回饋空氣品質模式使用經驗、程式編譯及測試結果予研發中心，提供模式未來精進的改善方向。也提供本署未來空氣品質動力模式之版本升級、耦合高解析度氣象數值預報模式及偏差修正等先進技術之交流平臺，並作為空氣品質預報作業自動化之精進參考。美國國家氣象局空氣品質格點預報系統（National Air Quality Forecast Capability, NAQFC）已於 2016 年 2 月進行 CMAQv4.6 版本的高解析度模擬，藉由垂直解析度的提升（由 22 層增加至 35 層)，提升臭氧和細懸浮微粒預報準確度。建議本署可針對利用高污染事件個案之高解析度重分析模擬測試（水平或垂直解析度提高或不同版本的測試)，分析 CMAQ 預報能力之差異，可做為未來於中央氣象局之作業化空氣品質模式網格配置設定的參考。

目錄

壹、目的及背景說明

我國環境保護署全年無休提供民眾空氣品質預報服務，每日上午 10 時 30 分及下午 4 時 30 分發布未來 3 天及外島隔日空氣品質預報。為增進空氣品質預報動力模式模擬之技術提升，需借鏡國外空氣品質預報作業模式之維運與發展技術，提供本署未來空氣品質動力模式之版本升級，耦合氣象數值預報模式及偏差修正等先進技術之交流平臺。

美國環境保護署與北卡羅萊納大學教堂山分校（The University of North Carolina at Chapel Hill, UNC-CH）自 2003 年起共同成立空氣品質模式研發中心 (Community Modeling and Analysis System，CMAS），過去 15 年來每年召開的年度研討會，已成為先進空氣品質模式研討的最佳交流平臺。CMAS 模式研發中心致力於發展及推廣由美國環境保護署推動的第三代空氣品質模式（Community Multi-Scale Air Quality modeling system，CMAQ）。CMAQ 模式的模擬模組中不僅模擬氣態污染物，同時也處理懸浮微粒，並加入沉降作用的模擬，使模擬的面向更完整。第 15 屆空氣品質模式發展研討會(15th Annual Community Modeling and Analysis System Conference）於 105 年 10 月 24 至 26 日在美國北卡羅萊納州教堂山星期五會議中心（Friday Center）召開，參與的環境部門代表及學術研究人員分別來自美國、加拿大、巴西、哥倫比亞、中國大陸、印度、法國、日本及臺灣等共計 13 個國家，各國代表及專家學者透過研討交流，回饋模式使用經驗、程式編譯及測試結果予 CMAS 研發中心，提供 CMAQ 模式未來精進的改善方向。

貳、研習過程

此次行程始於 105 年 10 月 23 日上午台北起程飛往美國洛杉磯，再轉機前往北卡羅萊納州羅利德罕機場，於當地時間晚間抵達研討會召開地點北卡羅萊納州教堂山。本次研討會自 10 月 24 至 26 日為期 3 天進行，口頭（Oral）報告共有 104 篇，海報論文發表共有 48 篇，共計 152 篇。論文其中以來自美國占多數，達 123 篇，日本 9 篇，加拿大 8 篇，台灣 3 篇；澳洲 4 篇；英國 3 篇；法國 1 篇；中國 1 篇。18 個議程涵蓋空氣品質模式發展、先進氣象模式近期改善與發展、高解析模式模擬應用、模式個案診斷分析、氣象場對空氣品質模式準確度之敏感度測試、全球與區域模式運用、氣候變遷與能源等議題（附錄二），可供本署空

氣品質預報技術發展之參考。

研討會第1天開幕式首先由北卡羅萊納大學 Adel Hanna教授，同時兼任CMAS主席進行開幕致詞 ，介紹CMAS中心自2003年成立以來，致力的空氣品質模式的研發，並建立完整的技術交流與軟體教育訓練的國際推廣平臺（附錄三）。Keynote演說分別為美國海洋及大氣總署（NOAA）Gregory Frost博士介紹大氣污染排放資訊更新技術的新挑戰（附錄四）及賓州大學David Stauffer教授介紹先進氣象模式在資料同化最新發展（附錄五）。研討會第2天議程主題為CMAQ模式最新發展、源解析診斷及小區域精緻化模擬分析及應用等32場演講。首先由美國環保署大氣模式發展小組Jon Pleim博士介紹CMAQ最新5.2版本在大氣化學機制的更新及展望下一代空氣品質模式的方向（附錄六）。下午為論文海報解說時段，計有42篇論文海報參加，其中中央大學大氣物理所鄭芳怡教授有2篇有關於臺灣雲林縣細懸浮微粒（$PM_{2.5}$)診斷分析，透過CMAQv5.0.2版本之水平網格3公里高解析度模擬及敏感度實驗，診斷分析臺中火力發電廠及麥寮工業區對雲林地區高污染事件的貢獻（附錄七）。

研討會第 3 天議程主題為模式個案診斷分析及氣象初始場模式之敏感度測試。其中中央大學莊銘棟教授講題為定量探討細懸浮微粒透過東亞冬季季風長程輸送至臺灣地區的貢獻。另外 NOAA 的 Jeff McQueen 博士報告美國國家氣象局空氣品質格點預報系統（National Air Quality Forecast Capability, NAQFC）已於 2016 年 2 月進行 CMAQv4.6 版本的高解析度測試，初步評估在臭氧和細懸浮微粒預報準確度有相當程度的改善，未來線上作業模式將更新為 CMAQv5.0.2 版本，以來改善 $PM_{2.5}$ 的預報技術得分（附錄八）。

參、心得與建議事項

本次出國主要目的為學習美國先進空氣品質動力模式耦合高解析度氣象數值模式（CMAQ-WRF)之方法，進一步運用先進偏差修正技術（Bias correction)，了解如何客觀校驗空氣品質模式的準確度，藉由技術交流過程提供本署空氣品質預報作業自動化之精進參考。

一、CMAQ 模式從第 5 版之後，針對 $PM_{2.5}$ 模擬的化學機制有更完善的參數化過程。美國國家氣象局 NAQFC 系統，每日提供 0600 UTC 及 1200 UTC 2 次

全美地區的未來 48 小時空氣品質格點預報資訊，模式結果輸出時間分別為 1300 UTC 及 1730 UTC。2016 年 2 月已將 NAQFC 系統中 CMAQv4.6 版，垂直解析度由 22 層增加至 35 層，最細層網格水平解析度為 12 公里 。$PM_{2.5}$ 夏季預報有低估趨勢，準確度約 0.67 至 0.74；冬季準確度有高估趨勢約 0.58 至 0.64，藉由解析度提升，整體誤差可減少 52%，未來 NAQFC 也將提升為 CMAQv5.0 版本。有關 NAQFC 線上校驗可參考 NOAA 相關網站查詢（http://www.emc.ncep.noaa.gov/mmb/aq/），該網頁顯示介面可供未來線上即時校驗系統建置之參考。另建議本署可針對利用高污染事件個案之高解析度重分析模擬測試（水平或垂直解析度提高或不同版本的測試），分析 CMAQ 預報能力之差異，可做為未來於中央氣象局之作業化空氣品質模式網格配置（domain configuration）設定的參考。

二、本署輔助空氣品質預報系統作業化模式為 CMAQv4.6 版，考量 $PM_{2.5}$ 模擬的準確度，建議未來亦提升為 CMAQv5.0 以上版本。另外，有關複雜地形的空氣品質模擬，在本次研討會也有相關論文探討。例如美國加州因西臨太平洋、東側洛磯山脈縱貫及灣流（舊金山灣區）等複雜地形，造成局部小尺度環流及氣膠海氣交互作用的機制較美國中西部平原地區之大尺度環流複雜，也導致加州地區空氣品質模擬準確度較差（附錄九）。類似情形也發生在被中央山脈縱貫全島的臺灣地區，故建議本署 CMAQ 模式介接交通部中央氣象局 45 層高垂直解析之作業化 WRF 氣象模式為預報邊界初始資料，藉由提高局部小尺度環流之氣象場掌握度來提升臺灣複雜地形的空氣品質預報準確度。

三、美國國家氣象局 NAQFC 系統應用卡曼濾波器（Kalman filter）先進偏差修正技術，有效縮小 $PM_{2.5}$ 預報誤差，並改善 48 小時預報準確度，對外發布更為準確的美國本土地區 $PM_{2.5}$ 48 小時格點預報資料產品。相關技術可最作為本署未來空氣品質模式輸出統計方法模型建置、預報校驗工具開發及預報作業自動化之精進參考。本署輔助空氣品質預報系統已運用 Decaying average 技術進行系統性偏差修正，目前在臭氧的預報修正表現比 $PM_{2.5}$ 佳，建議 $PM_{2.5}$ 部分未來可應用卡曼濾波器偏差修正技術。

附錄一　研討會相關照片

圖 1 研討會會場，UNC Friday Center

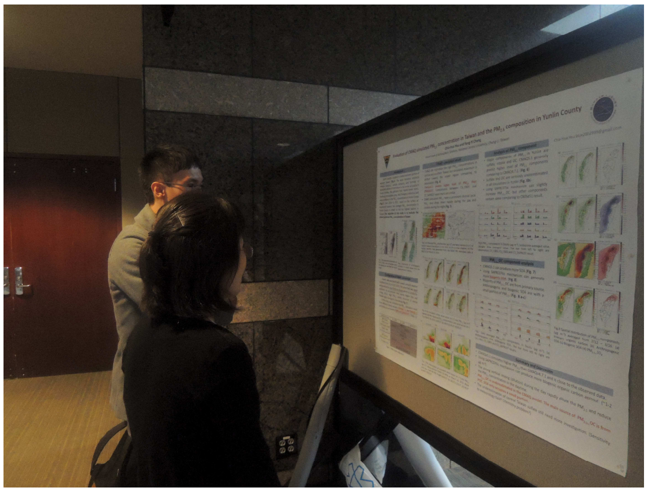


圖 2　論文海報講解情形

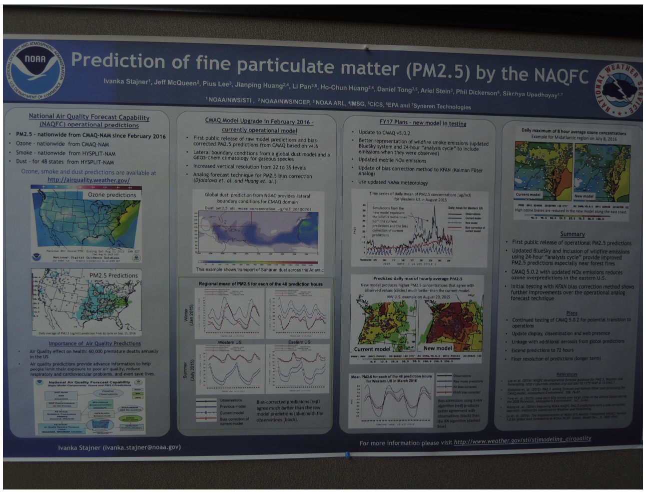


圖 3　美國氣象局 NAQFC 空氣品質格點預報系統 $PM_{2.5}$ 預報論文海報說明

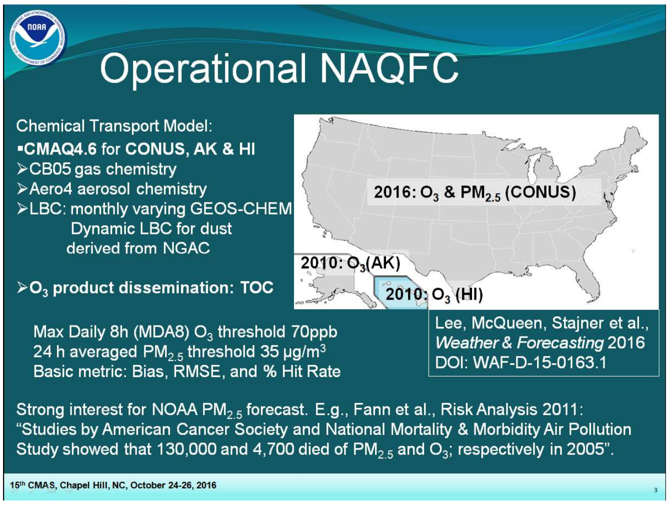
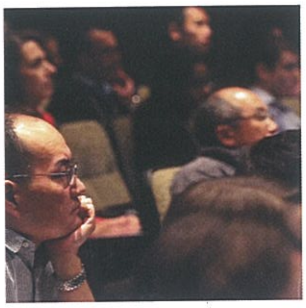
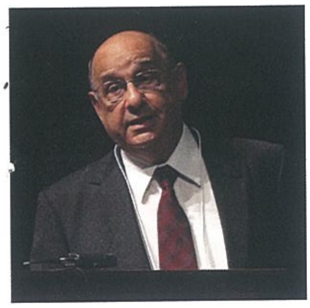


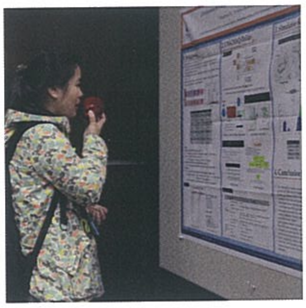
圖 4　NAQFC 目前預報作業化現況

附錄二　議程

2016 CMAS Conference







15 celebrating *years* of CMAS

Oct. 24-26 | Chapel Hill

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WELCOME

Welcome to the 15th annual CMAS conference. CMAS conferences have become a popular platform to learn about advancements in air quality modeling.

The United States Environmental Protection Agency (EPA) has collaborated with several leading researchers in atmospheric modeling and software infrastructure to establish the non-profit CMAS Center to support the air quality modeling user community in the U.S. and abroad. The University of North Carolina at Chapel Hill (UNC) has been the host of the CMAS Center through competitively awarded, successive multi-year EPA contracts since its inception.

The CMAS Center is a functional entity, providing expertise in support of open-source, public domain air quality model products. UNC has developed an exemplary reputation as the host of the CMAS Center over the past 15 years. The CMAS community includes over 5,000 participants from around the world. The community of CMAS users includes regulatory, academia, federal, state, and local governments, industry, consultants, and international users from 90 countries. The CMAS website (www.cmascenter.org), with its multiple model component links, is a well-known information hub for air quality modelers seeking software, data, support, and training. For over a decade, UNC's CMAS Center has managed over 100 releases of 14 open-source modeling and analysis tools including CMAQ, SMOKE, AMET, MCIP, BenMAP, I/O API, Spatial Allocator, VERDI, FEST-C, R-LINE, and C-LINE – all critical tools for a global air quality modeling community. The CMAS help desk provides technical guidance from software developers and expert users to address questions on the CMAS software from the user community.

UNC has established in the CMAS Center a dynamic education and outreach program that includes workshops, training, a visiting scientist program, annual conference(s), and a robust record of peer-reviewed publications. Over the past decade, in collaboration with EPA, UNC has organized more than 11 workshops on specific topics of scientific interest. Among these is the biannual CMAQ review, the fifth of which was conducted in the summer of 2015. The CMAS training program is highly regarded by the user community, and has trained more than 3,000 users from the U.S. and abroad, at no cost to EPA. A major benefit of the conference has been CMAS Center's coordination with leading environmental and air quality journals to publish special issues of selected, peer-reviewed papers from the conference presentations. The CMAS Center engages a broad spectrum of community members, spanning academia, government, and private industry to serve on its EAC and provide guidance on ways to improve the CMAS support services to the user community. Through the CMAS Visiting Scientist program, UNC hosts scientists on extended visits (from one month to a year) to study or develop modeling components and methods in collaboration with CMAS and EPA scientists. CMAS also publishes an electronic newsletter to connect community members with system information, model updates, and upcoming events.

The third South America CMAS conference is planned for Brazil next year. Aug. 2017

I hope you enjoy your time at this 15th annual conference and celebration!

Adel Hanna
Director | Center for Environmental Modeling for Policy Development

October 24, 2016

	Grumman Auditorium	
7:30 AM	Registration and Continental Breakfast	
8:00 AM	A/V Upload	
8:30 AM	**Welcome and Opening Remarks**	
8:45 AM	**CMAS Status Update, Adel Hanna (UNC)**	
	Plenary Session: "Emerging Issues in Air Quality Modeling" Chaired by Rohit Mathur (US EPA) and Jon Pleim (US EPA)	
9:00 AM	**Understanding and improving emissions information through atmospheric observations** Gregory J. Frost (NOAA)	
9:30 AM	**Advances in meteorological modeling and data assimilation** David R. Stauffer (Penn State)	
10:00 AM	Break	
10:30 AM	**How do we improve the treatment of atmospheric chemistry in future air quality models?** Deborah Luecken (US EPA)	
11:00 AM	**Atmospheric aerosol modeling needs for next generation air quality models** Michael Kleeman (UC Davis)	
11:30 AM	**Air quality and chemistry-climate interactions: emerging research in land surface models** Gordon Bonan (NCAR/UCAR)	
12:00 PM	Lunch in Trillium	
	Grumman Auditorium **Air Quality, Climate, and Energy** Chaired by Mike Barna (NPS) and Will Vizuete (UNC)	**Dogwood Room** **Emissions Inventories, Models and Processes** Chaired by Tom Pierce (US EPA) and BH Baek (UNC)
1:00 PM	Opportunities for Reducing Vegetative Ozone Exposure through U.S. Power Plant Carbon Standards Shannon Capps	Developments in the 2014 National Emissions Inventory Rich Mason
1:20 PM	Impacts of Technology-Driven Transportation Emissions on Future U.S. Air Quality in a Changing Climate Patrick Campbell	Development of 2011 Hemispheric Emissions for CMAQ Alison Eyth
1:40 PM	Impact of the Biomass Burning Aerosols on the Regional Climate of the Southeastern U.S. Peng Liu	Emissions Reconciliation Analyses in Californias South Coast Air Basin Stephen Reid
2:00 PM	Air Quality Impacts of Electrification in tandem with Intermittent Renewable Resources Michael MacKinnon, Ph.D.	Incorporate Traffic Demand Model Data in SMOKE-MOVES Processing for

		Denver Ozone Modeling Tejas Shah, Ramboll Environ, Novato, CA
2:20 PM	Break	Break
2:50 PM	Air Pollution Externalities and Energy Choices: Linking Electricity Dispatch, Air Quality and Health Impact Models Michael D. Moeller	Development of an Emission Uncertainty Inventory and Modeling Framework: Case Study of Residential Wood Combustion Rabab Mashayekhi
3:10 PM	Quantifying the effect of natural variability on the assessment of climate policies' health benefits compared to costs Rebecca K. Saari	SPATIAL DISTRIBUTION OF PARTICULATE MATTER EMISSION FROM RESIDENTIAL COMBUSTION IN LATIN AMERICA, AFRICA, AND ASIA Ekbordin Winijkul
3:30 PM	Modeled Source Apportionment of Reactive Nitrogen in the Greater Yellowstone Area Mike Barna	A combined line-point-source model for ship emissions in the port of Hamburg, Germany Armin Aulinger
3:50 PM	Quantifying co-benefits of CO2 emission reductions in Canada and the US: An adjoint sensitivity analysis Marjan Soltan Zadeh	Improving Air Quality Modeling Performance and Capabilities in Bogot, Colombia Pachon, Jorge

Poster Session 1

Air Quality, Climate and Energy

1) Estimating source attribution from oil and gas extraction on nitrogen deposition at western national parks using CAMx-PSAT
Michael Barna

2) Impacts of climate change on photochemical pollutants and allergenic pollen in the United States
Ting Cai, Allison P. Patton

3) Concentrations of individual fine particulate matter components in the United States around the 4th of July
Elizabeth Chan

4) Association of trends in US ambient air quality and cardiovascular mortality for 2000-2010
Anne E Corrigan

5) Exposure to Fine Particulate, Black Carbon, and Particle Number Concentration in Transportation Modes in Bogota
Boris Galvis

6) Studying Aerosol Indirect Effects on Grid and Subgrid Scale Clouds using the two-way Coupled WRF-CMAQ
Jian He

7) Development of the GAINS-Korea for Integrated Assessment of Greenhouse gas ? Air pollutant Management in Korea
Younha Kim

8) Real-Time Air Quality Forecasting over Southeastern United States using Updated Emissions and Satellite-Constrained Boundary Conditions

Qi Li

9) Effects of aerosol feedback on aircraft-attributable surface O3 and PM2.5 concentrations using the two-way coupled WRF-CMAQ modeling system
Chowdhury Moniruzzaman

10) Estimating Environmental Co-benefits of U.S. GHG Reduction Pathways Using the GCAM-USA Integrated Assessment Model
Yang Ou

11) Incorporating Air Pollutant Emission Factors and State-Level Controls and Energy Policies within the GCAM-USA Integrated Assessment Model
Wenjing Shi

12) Development of GUIDE (GHG and air pollutants Unified Information Design system for Environment) system
Jung-Hun Woo

13) Exploring Conditions Leading to Wintertime Ozone Episodes in Natural Gas Fields
Yuling Wu

14) Air Quality and Acid Deposition Forecast of South Athabasca Oil Sands Development Applying CMAQ Model
Wen Xu

Emissions Inventories, Models, and Processes

4:10 - 5:45 PM

15) Development of an activity-based marine emission inventory using AIS data
Bruce Ainslie

16) Use of SMOKE model outside of USA: Mobile sources emission inventory using area type approach.
Igor Baptista

17) MEGAN vs BEIS in Texas: A biogenic model showdown
Doug Boyer

18) Effects of including nitrogen oxides emissions due to lightning on CAMx model performance in Texas
Shantha Daniel

19) Improved wildfire smoke modeling, AIRPACT-Fire, for enhanced communication of human health risk
Yunha Lee

20) An analysis of sensitivity of MOVES emissions estimates to traffic data and comparison to grid-cell estimates and near-road measurements from the Las Vegas field study
R. Chris Owen

21) The 2014 National Emission Inventory for Rangeland Fires and Crop Residue Burning
George Pouliot

22) THE 2013 CANADIAN AIR QUALITY MODELLING PLATFORM AND THE BASE FUTURE CASES USED FOR POLICY REGULATIONS
Mourad Sassi

23) Incomplete sulfate aerosol neutralization despite excess ammonia in the eastern US: a possible role of organic aerosol
Rachel Silvern

24) The predicted impact of VOC emissions from Marijuana cultivation operations on ozone concentrations in Denver, CO.
Chi-Tsan Wang

25) High-resolution emission inventories of agricultural fugitive dust in China
Aijun Xiu

26) Development of Current and Future-year Point Source Air Emissions Inventories for Alberta Province of Canada
Fuquan Yang

27) Development of 2014 Georgia Wildland Fire Emission Inventory
Tao Zeng

28) Canadian Anthropogenic Methane and Ethane Emissions: A Regional Air Quality Modeling Perspective
Junhua Zhang

Model Development

29) THE MODEL FOR SIMULATING THE ROCKET EXHAUST FORMATION AND DISPERSION AND ITS INTEGRATION WITH CMAQ FOR LONG RANGE ASSESSMENT
Taciana Toledo de Almeida Albuquerque

30) Implementation of Canopy Reduction mechanism to CMAQ
Jan A. Arndt

31) Lightning NOx Production in CMAQ: Part II - Parameterization Based on Relationship between Observed NLDN Lightning Strikes and Modeled Convective Precipitation Rates
Daiwen Kang

32) Application of novel particle formation and growth schemes in CMAQ
Benjamin N. Murphy

33) Halogen chemistry in the CMAQ model
Golam Sarwar

October 25, 2016

	Grumman Auditorium	Dogwood Room
7:30 AM	Registration and Continental Breakfast	
8:00 AM	A/V Upload	A/V Upload
	Model Development Chaired by Havala Pye (US EPA) and Jesse Bash (US EPA) A new version of the Community Multiscale Air Quality	**Regulatory Modeling and SIP Applications** Chaired by Taciana Albuquerque (UFMG in Brasil) and Byeong Kim (GA DNR) Predicting PM2.5 Concentrations that

8:30 AM	Model: CMAQv5.2 Jon Pleim	Result from Compliance with National Ambient Air Quality Standards James Kelly
8:50 AM	Enhancements to an Agriculture-land Modeling System - FEST-C and Its Applications Ellen Cooter	Source apportionment of biogenic contributions to ozone formation over the United States Daniel Cohan
9:10 AM	Lightning NOx Production in CMAQ: Part I - Using Hourly NLDN Lightning Strike Data Daiwen Kang	Dynamic Evaluation of Modeled Ozone Response to Emission Changes and Improvement of Future Year Ozone Projections in the South Coast Air Basin Prakash Karamchandani
9:30 AM	Updates on Soil NOx parametrization in CMAQ v5.1 Quazi Ziaur Rasool	Assessment of Intrastate Contributions to Ozone Nonattainment Monitors in Atlanta, GA Byeong-Uk Kim
9:50 AM	Break	Break
10:20 AM	Enhancements to Land Surface Processes for WRF/CMAQ with PX LSM Limei Ran	Source apportionment of fine particulate matter in Yunlin County in Taiwan Yi-Ju Lee
10:40 AM	A new physically-based windblown dust emission parametrization in CMAQ Hosein Foroutan	Modeling the Impacts of Prescribed Burns for Dynamic Air Quality Management M. Talat Odman
11:00 AM	Direct Radiative Effect of Dust Aerosols and Biomass Burning Over East Asia Xinyi Dong	Improving Regional PM2.5 Modeling along Utahs Wasatch Front Chris Pennell
11:20 AM	Updating CMAQ secondary organic aerosol properties relevant for aerosol water interactions Havala Pye	Predicting the Impact of a Wood-Stove Change-Out Program on Ambient Particle Levels in Utah's Airshed Nancy Daher
11:40 AM	Impacts on Ambient Particulate Matter by Changing Particle Size Distribution from Emissions Using the Community Air Quality Model (CMAQ): A Case Study of Commercial Aircraft emissions from Landing and Take-off Jiaoyan Huang	ASSESSMENT OF CURRENT AND FUTURE IMPACTS OF AIR POLLUTION ON HUMAN HEALTH Peter Suppan
12:00 PM	Lunch in Trillium	
	Model Development, cont.	**Fine Scale Modeling and Applications** Chaired by James Kelly (US EPA)
1:00 PM	Recent Updates made for SMOKE version 4.0 BH Baek	Comparison of human exposure model estimates of PM2.5 exposure variability using fine-scale CMAQ simulations from the Baltimore DISCOVER-AQ evaluation Janet M. Burke
1:20 PM	Organic Aerosol Sources and Partitioning in CMAQv5.2 Benjamin N. Murphy	Assessing the impact of grid resolution on forward and backward sensitivity results Melanie Fillingham
1:40 PM	CAMx Overview and Recent Updates Christopher Emery	Local to regional scale modeled wildland fire impacts on O3 and PM Kirk Baker
	Development and Applications of Next-Generation	Assessment of Air Quality Impacts from

2:00 PM	Integrated Air Quality Decision Support System (ABaCAS) Carey Jang	the 2013 Rim Fire Matthew Woody
2:20 PM	Break	Break
2:40 PM	Evaluation of a pending upgrade of the CTM of NAQFC from CMAQ version 4.6 to 5.0.2 together with a refined treatment to initialize wildfires-related PM Pius Lee	STILT-ASP: A Trajectory-Based Modeling Tool for Assessing the Impacts of Biomass Burning on Air Quality Christopher M. Brodowski
3:00 PM	Aerosol Assimilation Based on NCEPs GSI using Surface PM2.5 and Satellite AOD Youhua Tang	Modeling Single Source Secondary Impacts with the Higher-Order Decoupled Direct Method of Sensitivity Analysis Christopher Emery
3:20 PM	In-Line Coupling of the NMMB and CMAQ Models through NCEPs ESMF and NUOPC Framework Barry D. Baker	Recent Improvements to SCICHEM and Comparison of SCICHEM Single-Source Impacts with Photochemical Grid Models Prakash Karamchandani
3:40 - 5:15 PM	**Poster Session 2**	
5:30 - 8:00 PM	**Reception at NC Botanical Gardens**	

Poster Session 2 listing:

ABaCAS Demonstration given by Carey Jang

Fine Scale Modeling and Applications

1) Construction of Multi-fan Wind Tunnel for Radionuclides Atmospheric Dispersion
Haimin Fan

2) Different scale of eddy structures and their roles on pollutant dispersion in and over urban canopy layers
Yifan Fan

3) Characterization of Traffic Emissions Exposure Metrics in the Dorm Room Inhalation to Vehicle Emissions (DRIVE) Study
Jennifer Moutinho

4) Fine-Scale WRF/Chem Simulations over the Western U.S. for the Assessment of Future Technology-Driven Air Quality
Michael Pirhalla

5) Use of CMAQ for the 2011 National Air Toxics Assessment (NATA)
Madeleine Strum

6) Modeling prescribed fire impacts on local to regional air quality and potential climate effects
Luxi Zhou

Global/Regional Modeling Applications

7) Effect of global emissions on photochemical air quality in the Lower Fraser Valley Canada
Golnoosh Bizhani

8) Highlights from the Third Phase of the Air Quality Model Evaluation International Initiative (AQMEII3)
Christian Hogrefe

9) Relative impact of the projected emissions from industry and transportation on regional air quality in Ontario
L. Huang

10) Decadal Application of WRF/Chem under Current and Future Climate/Emission Scenarios: Part II. Impact of Projected Climate and Emission Changes on Future Air Quality over the U.S.
Chinmay Jena

11) Prediction of harmful water quality parameters combining weather, air quality and ecosystem models with in-situ measurements
Catherine Nowakowski

12) Using a simple operational global aerosol model to provide dynamic chemical boundary condition for dust to the operational NAQFC
Youhua Tang

13) Prediction of fine particulate matter (PM2.5) by the National Air Quality Forecast Capability
Sikchya Upadhayay

14) Air quality real-time forecast before and during the G-20 Summit 2016 in Hangzhou with the WRF-CMAQ and WRF/Chem systems: Evaluation and Emission Reduction Effects
Yang Zhang

Model Evaluation and Analysis

15) CMAQ simulations for Ozone over Region of Great Vit?ria (Brazil): influence of boundary conditions
Dr. Taciana Toledo de Almeida Albuquerque

16) Recent updates to the CMAQ model evaluation tools and the new AMET version 1.3
K. Wyat Appel

17) Modeled PM2.5 and O3 contribution from lateral boundary inflow and wildfires
Kirk R Baker

18) VERDI Visualization of Geospatial Datasets
Jo Ellen Brandmeyer

19) EXPLORING PARALLEL PROCESSING OPPORTUNITIES IN AERMOD
George Delic

20) Continuous, Near Real-Time Application and Evaluation of WRF-CMAQ
Brian Eder

21) Lateral Boundary Contributions to Ozone Differ using Inert or Reactive Tracers
Chris Emery

22) Dynamic evaluation of CMAQ wet deposition estimates: Observed vs modeled trends from 2002-2012
Kristen Foley

23) Evaluation of PM2.5 concentration in Yunlin County in Taiwan
Chia-Hwa Hsu

24) Data Fusion of Air Quality Model Simulations and Ground-based Observations: Application over North Carolina, USA
Ran Huang

25) Impact of GOES Enhanced WRF Fields on Air Quality Model Performance
Maudood Khan

26) A Comprehensive Performance Evaluation of WRF/Chem version 3.7.1 over the Contiguous United States for 2008-2012
Mike Madden

27) Evaluation of a line source dispersion model, RLINE, using multi-year hourly pollution measurements in Detroit, MI.
Chad Milando

28) Strong Influence of Deposition and Vertical Mixing on Secondary Organic Aerosol Concentrations in CMAQ and CAMx
Qian Shu

29) Modeled Source Contributions to CO and NOy Concentrations during the DISCOVER-AQ Baltimore Field Campaign
Heather Simon

30) In-depth examination of emissions inventories to support EPA evaluation of modeled ambient nitrogen oxides (NOx and NOy).
Claudia Toro

31) Constraining Biogenic Secondary Organic Aerosol (BSOA) production in CMAQ during the SOAS Campaign
Petros Vasilakos

Regulatory Modeling and SIP Applications

32) Quantifying contributions to U.S. environmental inequality: an adjoint sensitivity analysis
Robyn Chatwin-Davies

33) Developing and Evaluating a Multi-Pollutant, Risk-Based Air Quality Management Strategy for the Upstate South Carolina Region
Andy Hollis

34) Source apportionment for sulfate aerosols over East Asia: Case study on the year of 2005
Syuichi ITAHASHI

35) Prototype air-water environmental system with linkage between meteorology/ hydrology/ air quality model system and watershed acidification model
Chunling Tang

36) Current and Future Mobile Source Contributions to Air Quality

Margaret Zawacki

Remote Sensing and Measurements Studies

37) Evaluating ammonia (NH3) predictions in the NOAA National Air Quality Forecast Capability (NAQFC) using ground-based and satellite-based measurements on a national scale
William Battye

38) Influence of the Bermuda High on interannual variability of summertime ozone in the Houston-Galveston-Brazoria region
Mark Estes

39) Quantification of emission sources apportionment to the concentration of PM2.5 in Temuco, Chile, using receptor model.
Ernesto Pino-Cortes

40) Estimating Daily Ambient PM2.5 Concentrations in Texas Using High Resolution Satellite Product
Xueying Zhang

Sensitivity of Air Quality Models to Meteorological Inputs

41) Impact of Meteorology on Dispersion Model Performance
Fatema Parvez

42) Sensitivity of Simulated Severe PM2.5 Pollution to WRF-CMAQ Model Configurations
Hikari Shimadera

43) Improving Cloud Prediction in WRF Through the use of GOES Satellite Observations for SIP Modeling
Andrew White

October 26, 2016

	Grumman Auditorium	Dogwood Room
7:30 AM	Registration and Continental Breakfast	
8:00 AM	A/V Upload	A/V Upload
	Model Evaluation and Analysis Chaired by Kristen Foley (US EPA) and Wyat Appel (US EPA)	**Remote Sensing and Measurements** Chaired by Roger Timmis, Environment Agency, UK
8:30 AM	Evaluation and Comparison of Fourteen Air Pollution Field Development Methods Regarding their Application in Exposure Assessment Haofei Yu	High resolution OMI satellite retrievals of tropospheric NO2 in the eastern United States Daniel L. Goldberg
8:50 AM	AQMEII3: the EU and NA regional scale program of the Hemispheric Trasport of Air Pollution Task Force Stefano Galmarini	Utilization of Geostationary Satellite Observations for Air Quality Modeling During 2013 Discover-AQ Texas Campaign Arastoo Pour Biazar
	Multi-model Comparison of Lateral Boundary	Source Influences on Ambient Ozone

9:10 AM	Contributions to Ozone Concentrations over the United States Peng Liu	Precursor Concentrations in the Colorado Front Range Shannon Capps
	Model Evaluation and Analysis, cont.	**Sensitivity of Air Quality Models to Meteorological Inputs** Chaired by Roger Timmis, Environment Agency, UK
9:30 AM	Preliminary Results of the Model Intercomparison Study in the Asia (MICS-Asia) Phase III Kan Huang	Recent Performance of the NOAA Air Quality Prediction System using CMAQ and the Impact of Driving Meteorology Jeff McQueen
9:50 AM	Evaluation of the Community Multiscale Air Quality (CMAQ) modeling system version 5.2 K. Wyat Appel	Impacts of WRF lightning assimilation on offline CMAQ simulations Nicholas Heath
10:10 AM	Break	Break
10:40 AM	**Developer/User's Meeting: Alternative Future Realities - Considerations for Modeling**	
12:00 PM	Lunch in Trillium	
	Model Evaluation and Analysis cont.	**Global/Regional Modeling Applications** Chaired by Jared Bowden (UNC) and Tanya Spero (US EPA)
1:00 PM	NOX emissions, isoprene oxidation pathways, vertical mixing, and implications for surface ozone in the Southeast United States Katherine R. Travis	Equatorward Redistribution of Emissions Dominates the Tropospheric Ozone Change, 1980-2010 J. Jason West
1:20 PM	Ongoing EPA efforts to evaluate modeled NOy budgets Heather Simon	Estimating age-segregated per-vehicle health benefits for the Canadian fleet Angele Genereux
1:40 PM	Top-Down Constraints on Emissions of NH3, NOx, and SO2 during the 2013 NOAA SENEX Campaign Matthew J. Alvarado	Evaluation of rainfall Intensity-Duration-Frequency (IDF) curves developed from dynamically downscaled regional WRF simulations Chuen Meei Gan
2:00 PM	Dynamic analysis: assessing CMAQs ability to capture air quality trends over a time period of changing emissions Lucas RF Henneman	Using Extreme Events to Compare USGS and NLCD Land Use Data Sets in WRF for Dynamical Downscaling Stephany Taylor
2:20 PM	Two Decades of WRF/CMAQ simulations over the continental United States: New approaches for performing dynamic model evaluation and determining confidence limits for ozone exceedances Marina Astitha	Using Response Surface Modeling (RSM) for the Task Force on Hemispheric Transport of Air Pollution (HTAP) Joshua Fu
2:40 PM	Decadal Application of WRF/Chem under Current and Future Climate/Emission Scenarios: Part I. Comprehensive Evaluation and Intercomparison with Results under the RCP 8.5 Scenario Kai Wang	Sensitivity of WRF Regional Climate Simulations to Choice of Land Use Dataset Megan S. Mallard
3:00 PM	Break	Break
	UDINEE: EVALUATION OF URBAN DISPERSION	Recent Updates to the Canadian

3:30 PM	MODELS AGAIN JU2003 DATA, AN INTERNATIONAL INITIATIVE S. GALMARINI	Operational Regional Air Quality Deterministic Prediction System Mike Moran
3:50 PM	Investigating Causes of CMAQ Under Predictions of Sea Salt Aerosol in the San Francisco Bay Area Su-Tzai Soong	Quantifying the contribution and analyzing the chemical reactions of long-range transport and local pollutants for PM2.5 in Taiwan under winter monsoon Ming-Tung Chuang
4:10 PM	Interactive model performance evaluation tools Doug Boyer	Ozone Source Apportionment Modeling to Support Policy Initiatives in the Eastern United States Kenneth Craig
4:30 PM	A THREAD PARALLEL SPARSE CHEMISTRY SOLVER FOR CMAQ 5.1 George Delic	Examining Changes to Extreme Temperatures and Precipitation Across the U.S. Through 2100 Tanya Spero
4:50 PM	Can machine learning features identify fitness of meteorology simulations for application to air quality? Robert Nedbor-Gross	Modeling green infrastructure land use changes on future air quality in Kansas City Yuqiang Zhang

附錄三　**CMAS Status Update**

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The Community Modeling and Analysis System

CMAS

15 Years Serving the Community

Adel Hanna

Director, CMAS

15th Annual CMAS Conference, October 2016

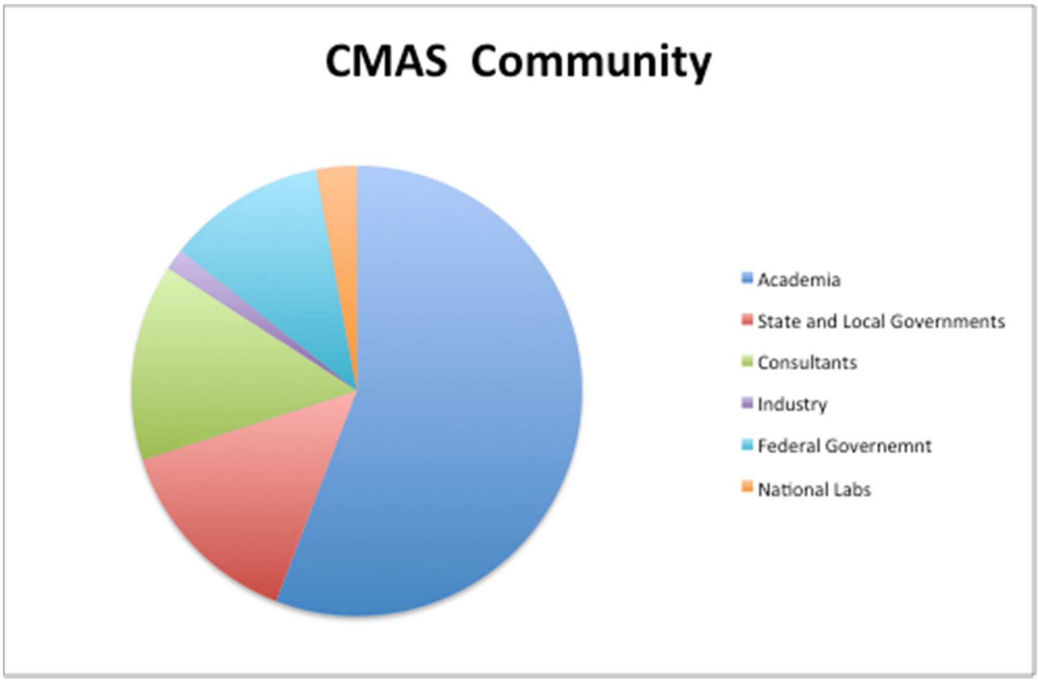
CMAS Center at UNC

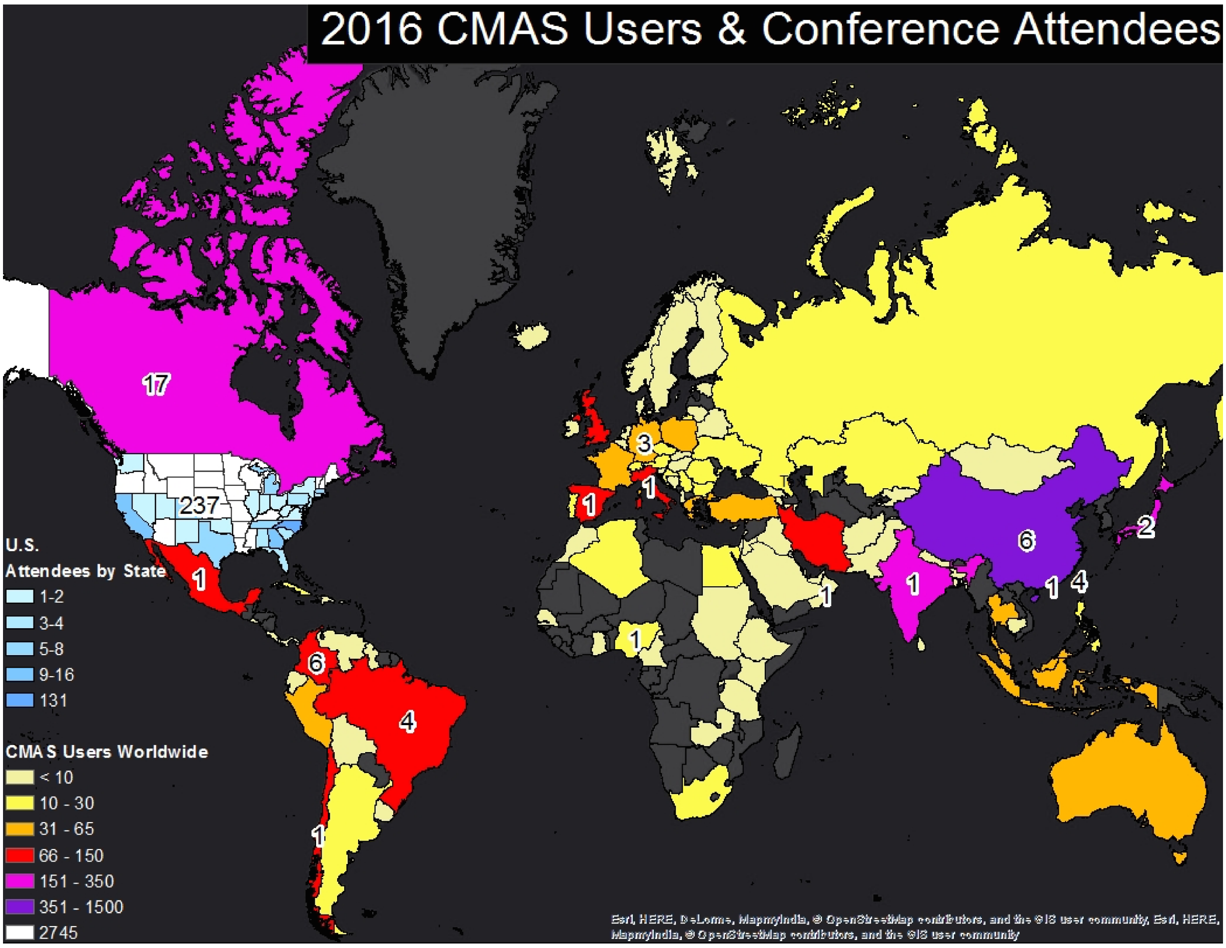
Established in 2001, the EPA's CMAS Center has been hosted at UNC since 2003, which works with the agency to lead the international, open-source, community-based air quality modeling and analysis software used to evaluate and propose regulations.

- Bridge between segments of the air quality modeling community
- Fosters growth of developer and user communities
- Hub for modeling education and training

CMAS Functions

- User Support
- Computational research and development
- Application and training
- Outreach


CMAS Community
Academia
State and Local Governments
Consultants
Industry
Federal Governemnt
National Labs


2016 CMAS Users & Conference Attendees
17
237
1
6
4
1
3
1
1
1
1
1
6
1
4
2
U.S.
Attendees by State
1-2
3-4
5-8
9-16
131
CMAS Users Worldwide
< 10
10 - 30
31 - 65
66 - 150
151 - 350
351 - 1500
2745
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Modeling and Analysis Tools

Model/Tool Released (This Year)

- Verdi 1.6 Alpha
- CMAQ 5.1
- C-Line 3.0
- I/O API 3.2
- MCIP 4.3
- FEST-C 1.2 with updates on the interface and EPIC model parameters
- Spatial Allocator (SA 4.2) – with updates on FEST-C tools, GOES satellite processing tools, and surrogate merging tool

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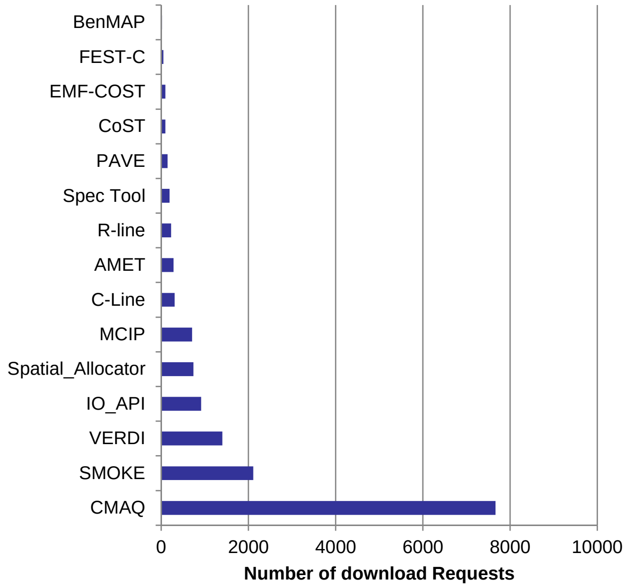
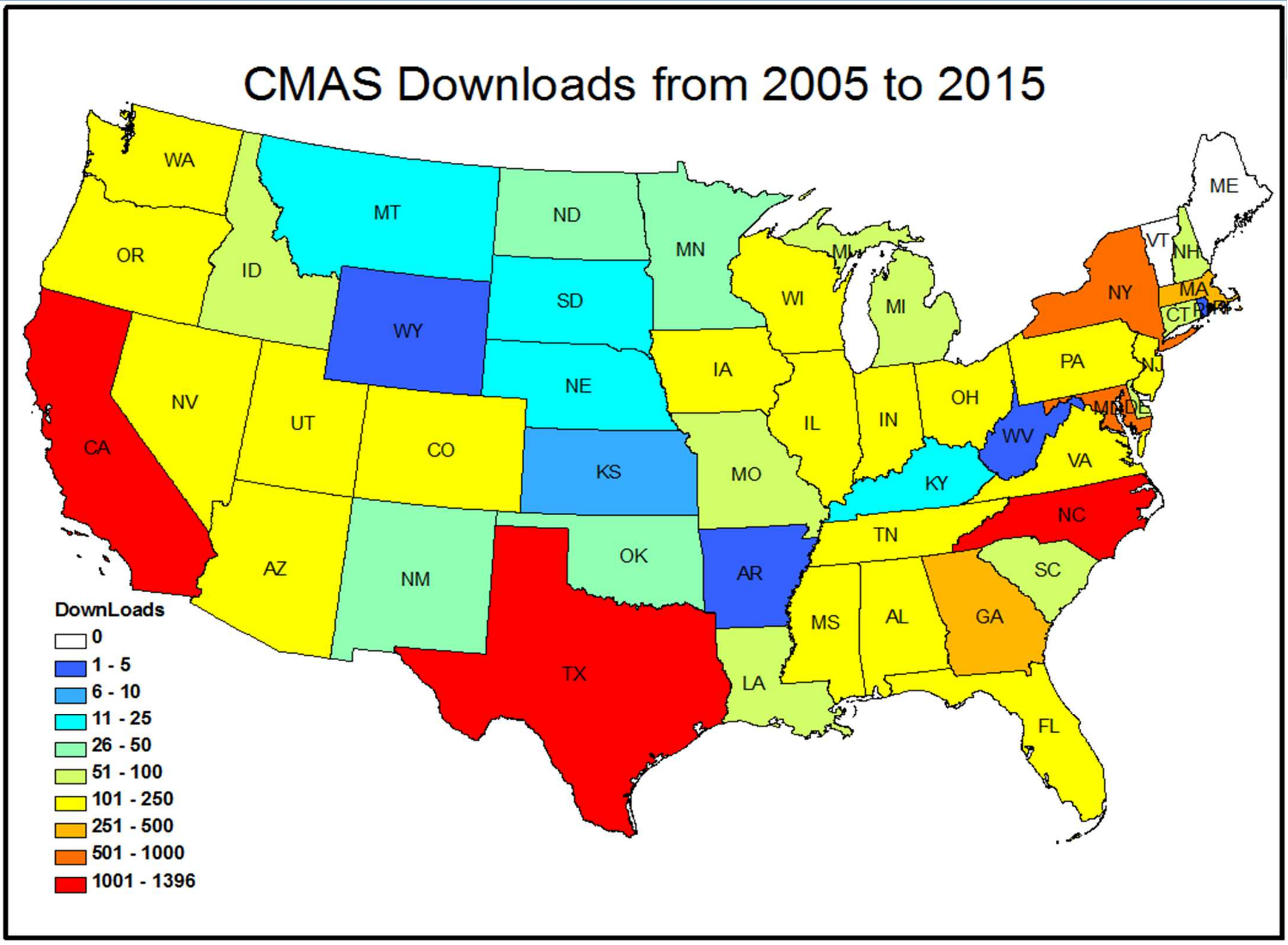
CMAS Product Downloads June 2015 – June 2016





CMAS Center at UNC - User Support

- Website-based internet support for users
- Email-based query system for questions/bugs
- Help desk as backup for web-based support
  - Technical and operational support: CMAQ, SMOKE, MCIP, Spatial Allocator, VERDI, AMET, BenMAP, R-LINE, C-Tools, FEST-C, and I/O API
  - New IT solutions tailored to specific functions of the CMAS Center
  - GitHub used for model source code and script distribution
  - Expand GitHub use to include “issues” feature for tracking bugs, new feature requests, and to-do lists for each CMAS-supported tool

User Support (II)

- Share model output data sets and other information
- Maintain on-line archive for model users
  - CMAS Data Exchange (CDX) to respond to CMAS user community
  - CDX will inventory air quality modeling data available in the community
  - Online resource available for the community to request and share meteorology, emissions, and air quality modeling data
  - CMAS is a member of ESIP

User Support (III)

- Maintain on-line archive for model users
  - Distribute CMAS software packages as both GitHub online archives and as stand-alone file archives
  - Work with EPA to develop high quality user and developer manuals

Computational Research an Development

Land-Atmosphere Fluxes

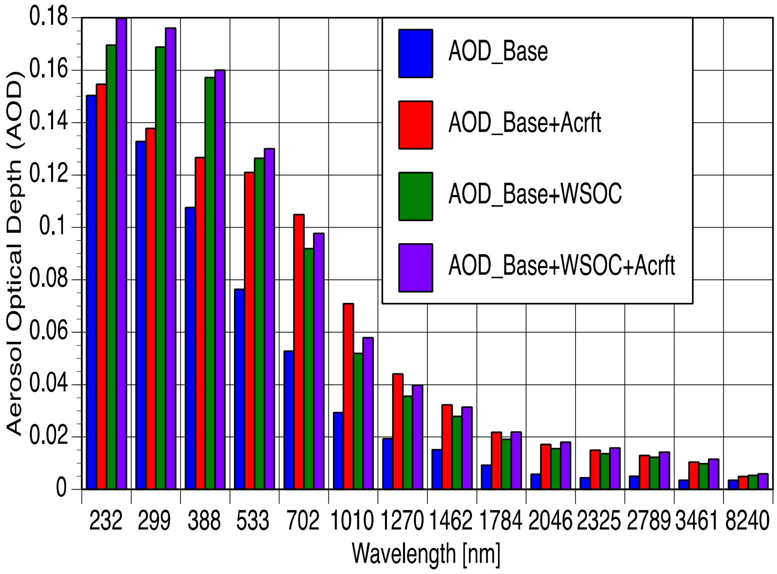
The **Fertilizer Emission Scenario Tool** for CMAQ **(FEST-C)** for CMAQ Bi-directional NH_3 Modeling

http://www.cmascenter.org/fest-c/

- FEST-C is a Java-based interface system which is used to simulate daily fertilizer application information for CMAQ domain grid cells within the US using the Environmental Policy Integrated Climate (EPIC) model.
- A required input for the CMAQ bi-directional NH_3 modeling is then extracted from the daily EPIC output.
- Spatial Allocator BELD4 tool which processes tiled MODIS land cover data (MCD12Q1) and with built 2001 and 2006 crop tables for US and Canada. To be used in the WRF/CMAQ consistently by EPA.
- Spatial Allocator Capability to compute surrogates for polygon shapefiles (e.g. census tracts)

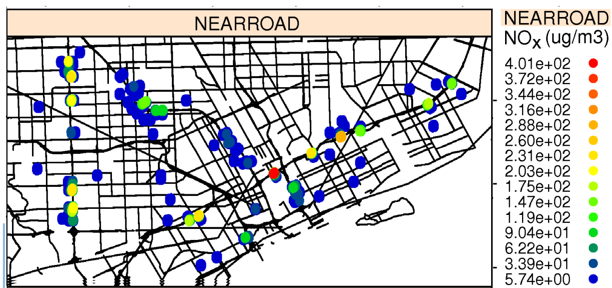
Computational Research and Development(II)
Radiative Effects of Aerosols

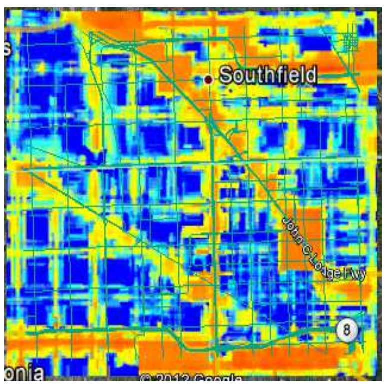
Reduce uncertainty in the modeling of the direct radiative effects of aerosols, by improving the representation of aerosol size distributions, chemical composition, and aerosol mixing state on which aerosol optical properties strongly depend.



Computational Research and Development(III)
Fine-Scale Modeling

- RLINE: EPA ORD's research dispersion modeling tool for near roadway assessments (*Snyder et al, 2013; Venkatram et al, 2013; Heist et al, 2013*)
- RLINE can support health and risk assessments, epidemiology studies, and community based tools
- UNC is developing C-LINE, a decision support tool for evaluating effects of alternate transportation options on community health

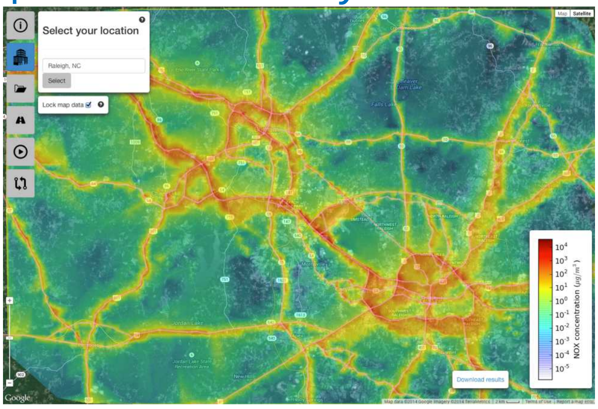




Community LINE Source Model (C-LINE)

https://www.cmascenter.org/r-line/

C-LINE is based on the R-LINE model
- Web-based easy-to-use GUI, with national coverage
- Model traffic-related near-road air pollution on-demand
- Back-end includes AERMET-based meteorology, FHWA Road Network/activity, and MOVES-based Emis. Factors
- Ability to change emissions or meteorological condition
  - Changes in fleet composition or activity
- Visualize absolute and relative changes in near-road air pollution
- CO, NO_x, $PM_{2.5}$, MSATs

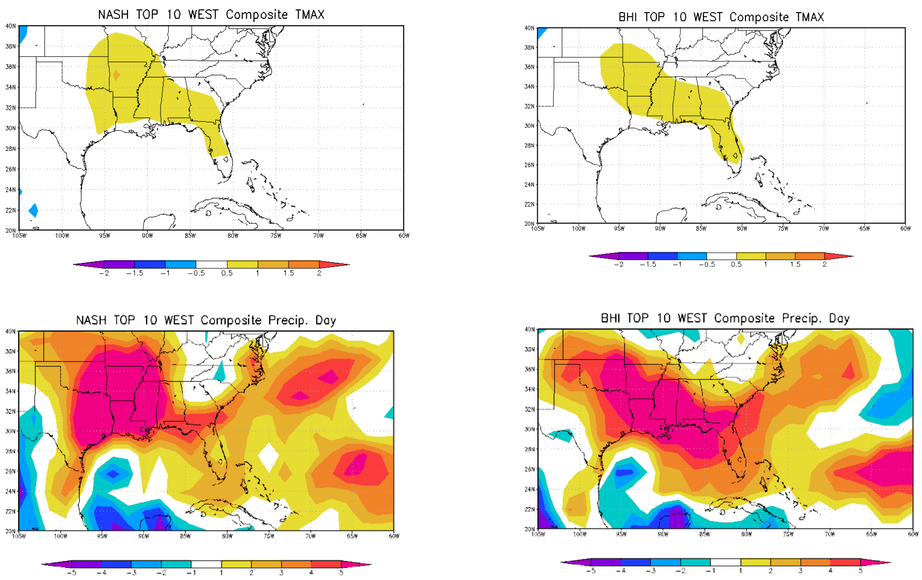


Computational Research and Development(IV) Regional Climate Change SE US

NASH Westward Shift | Most intense NASH

Temperature

Precipitation



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Applications and Training

- Training Sessions Onsite and Offsite
  - Two training sessions onsite at UNC
  - International (Hong Kong, Korea, Brazil, China, Columbia, Bulgaria, Canada, Greece, Mexico, India)
  - **SMOKE and CMAQ on-line training**
  - **Special Training; Python for Air Quality Research na Applications**

CMAS Training Sessions

Location	Date	Trainees
CMAQ		
Hong Kong University for Science and Technology	July 2015	15
Bogota, Colombia	August 2015	22
UNC Campus	October 2015	16
UNC Campus	April 2016	18
UNC Campus	October 2016	24
Total: CMAQ		***95***
Python for Air Quality Research and application		
UNC Campus		**26**
SMOKE		
Bogota, Colombia	August 2015	18
UNC Campus	October 2015	7
UNC Campus	April 2016	12
UNC Campus	October 2016	16
Total: SMOKE		***53***
SMOKE On-Line		
UNC-Campus	June 2015	20
UNC-Campus	February 2016	12
Grand Total		***206***

CMAS Promotes and facilitates collaboration and information sharing

- Conferences
  - 3rd CMAS South America Conference (Brazil, August 2017)
  - Student best poster
- Webinar series
- Listservs for community-based discussions
- CMAS wiki
- Visiting Scientists program
- Newsletter
- CMAQ peer review
- Peer reviewed journal articles
- Specialty workshops

Workshops

- Urban Database Planning Workshop (May, 2006)
- Panel review of CMAQ model process upgrades and model applications and evaluations (December, 2006)
- International conference on Atmospheric Chemical Mechanisms (December, 2008)
- Workshop for atmospheric modeling planning (July, 2008)
- CMAQ Adjoint Workshop (November, 2010)
- Meteorology-Hydrology Linkage Workshop (January, 2011)
- Panel review of the CMAQ model process applications, and evaluations (June, 2011)
- Workshop on integrated meteorology and chemistry modeling (October, 2012)
- Workshop on providing regional climate change projections for the southeastern US (April, 2013)

Main Conference Technical Events

- Plenary Session
  - Emerging Issues in Air Quality Modeling. Chaired by the U.S. EPA's Rohit Mathur and Jon Pleim
- CMAS Developer/User's Forum

  Alternative future realities: considerations for modeling

  Moderator, Tom Moore (WESTAR-WRAP); Panelists: Michael Barna (National Park Service - Air Resources Division), Chris Emery (Ramboll-Environ), Dan Loughlin (U.S. EPA), Tanya Spero (U.S. EPA)
- ABaCAS Software Demo. Carey Jang. U.S. EPA

  Air Benefit and Cost Attainment Assessment System (ABaCAS)

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CMAS Team at UNC

Applications and Training	***Zac Adelman***, B.H. Baek, Sarav Arunachalam, Uma Shankar, Alex Valencia, Liz Adams
Software Development	***Sarav Arunachalam***, Carlie Coats, Alex Valencia, Mohamed Omary, Jo Ellen Brandmeyer
Modeling Research	***Uma Shankar***, Frank Binkowski, Jared Bowden, Michelle Snyder,
Technical Editing	***Margaret Ledyard-Marks***
Communications and Events	***Brian Naess and Kathleen Clabby O'Rawe***
Director	***Adel Hanna***

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Thank You

- CMAS Community, EAC members, and Session Chairs
- Dr. Band for opening this conference
- UNC-Chapel Hill
- CMAS-EPA Project Manager (Thomas Pierce)
- Special Thanks To Dr. Bill Benjey (former CMAS-EPA Project Manager)

THE UNIVERSITY
of NORTH CAROLINA
at CHAPEL HILL

附錄四　**Understanding and improving emissions information through atmospheric observations**

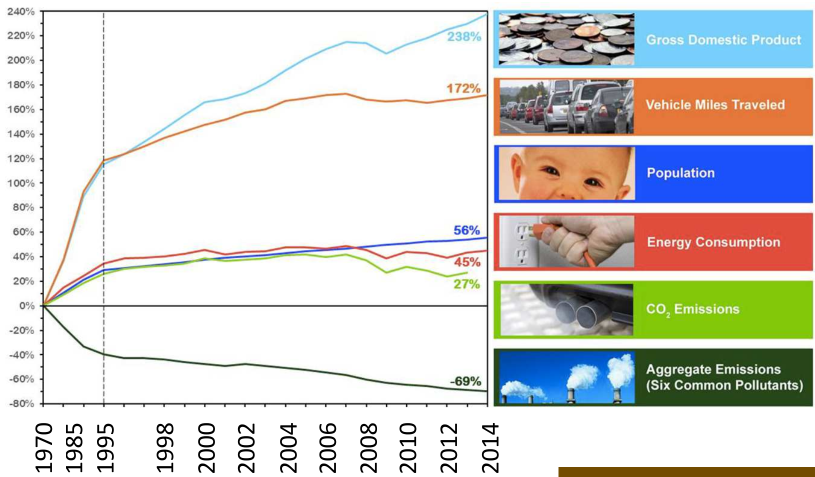
Understanding and improving emissions information through atmospheric observations and models

Greg Frost

Chemical Sciences Division, Earth System Research Laboratory
National Oceanic & Atmospheric Administration, Boulder, Colorado, USA
Gregory.J.Frost@noaa.gov, http://www.esrl.noaa.gov/

Acknowledgements: Ravan Ahmadov, Jessica Gilman, Joost de Gouw, Claire Granier, Si-Wan Kim, Brian McDonald, Megan Melamed, Paulette Middleton, Jeff Peischl, Gabrielle Petron, Tom Ryerson, Colm Sweeney, Christine Wiedinmyer

Successes and Challenges of US Clean Air Act

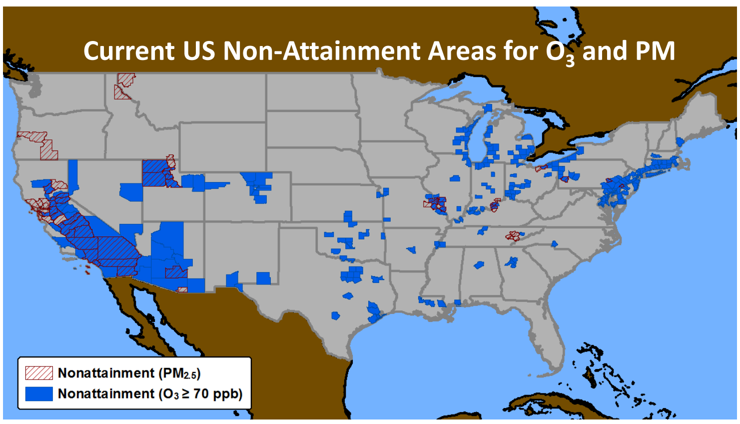


US Clean Air Act and subsequent regulations have reduced emissions of criteria pollutants for decades.

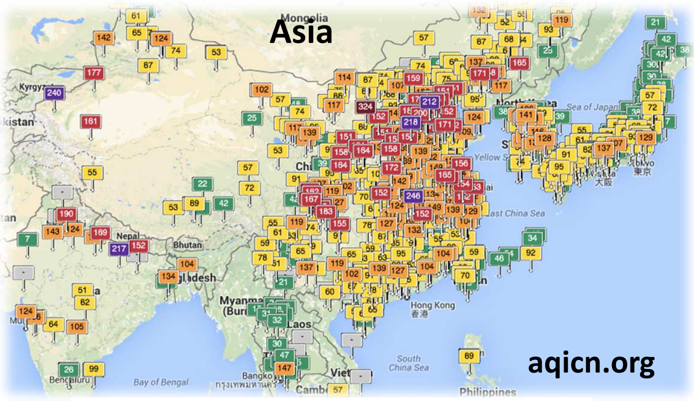
At the same time, population, economy, vehicle use, and energy consumption increased

www3.epa.gov/airtrends/aqtrends.html

US counties representing a significant fraction of US population remain in non-attainment of O_3 and PM standards



Global impacts of air pollution



Green: good **Yellow**: moderate
Red: unhealthy **Brown**: hazardous

- Bad air quality is still a serious issue in many parts of the world
- Air pollution is a leading cause of illness and mortality worldwide
- Other nations look to the US for guidance on understanding and solving these problems


World Health Organization

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Public health, environmental and social determinants of health (PHE)

Burden of disease from ambient and household air pollution

In new estimates released, WHO reports that in 2012 around 7 million people died - one in eight of total global deaths – as a result of air pollution exposure. This finding more than doubles previous estimates and confirms that air pollution is now the world's largest single environmental health risk. Reducing air pollution could save millions of lives.

Read the news release on air pollution attributable deaths
Read the feature story on air pollution
FAQs on air pollution and health
pdf, 169kb
Air pollution estimates
pdf, 1.16Mb
Summary of results and method descriptions

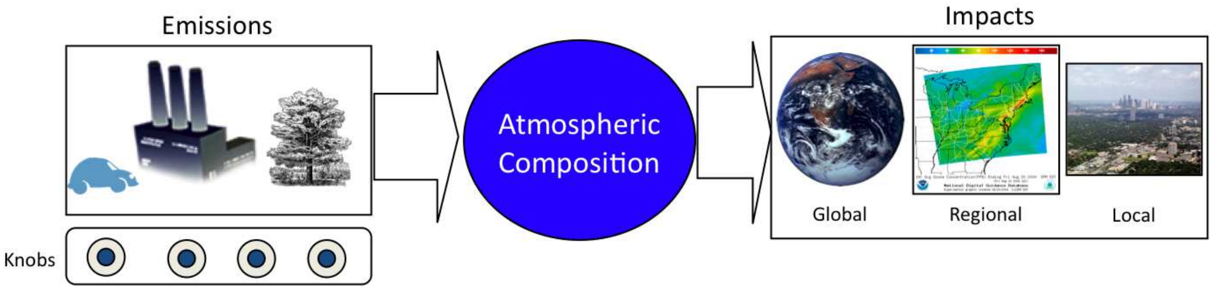
3.7 million deaths
attributable to ambient air pollution

4.3 million deaths
attributable to household air pollution

1600 cities
worldwide are reporting air pollution levels

www.who.int/phe/health_topics/outdoorair/

Environmental actions and decisions focus on emissions



Emissions data addresses multiple mandates and has many uses

Research
Analysis
Prediction
Long-range transport
Air quality
Climate change

Regulation
Atmospheric modeling
Human exposure
Permitting & compliance
Standards attainment
Public reporting

Economics
Emissions trading
Control implementation

Diplomacy
Assessments
Pollution conventions
Data sharing

Bottom-Up Inventory Methods

Inventories are simple in structure but complex in application

Total mass of compound X emitted

$$E_X = \Sigma_S [EF_{X,S} \bullet A_S \bullet (1 - CE_{X,S})]$$

Sum up all sources S

Emissions factor = mass of compound X emitted by source S per unit activity

Activity of source S, e.g., amount of fuel burned

Effectiveness of control measures for compound X at source S

Calculated for…
Specific region
Specific time
Also need…
Spatial allocation
Temporal variation
Speciation

Inventories are fundamental

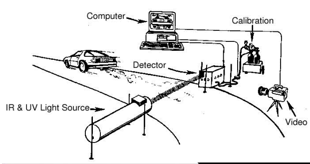
- Process-level understanding
- High granularity
- Comprehensive view
- Key model inputs
- Quantify changes
- Prediction
- Connect disciplines
- Key decision-making tools

Inventories face challenges

- Complexity
- Insufficient data
- Long costly development cycle
- Diverse data sources, traceability
- Proprietary data
- Inconsistencies
- Unknown or missing sources
- Super-emitting or sporadic sources
- Uncertainties difficult to estimate

Top-down Emissions Approaches

- Rely on high quality atmospheric observations of atmospheric abundance
- Use chemical-transport models of varying complexity to convert atmospheric abundance into emissions
- Hybrid approach: use atmospheric measurements in bottom-up inventory



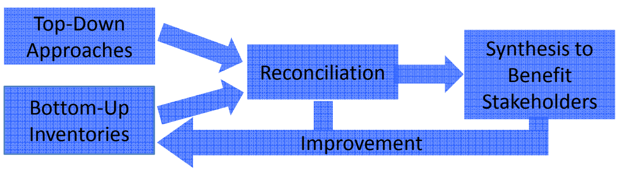
Top-down deliverables:

- Total emissions
- Spatial mapping
- Temporal variation
- Sector partitioning

Some benefits of top-down methods:

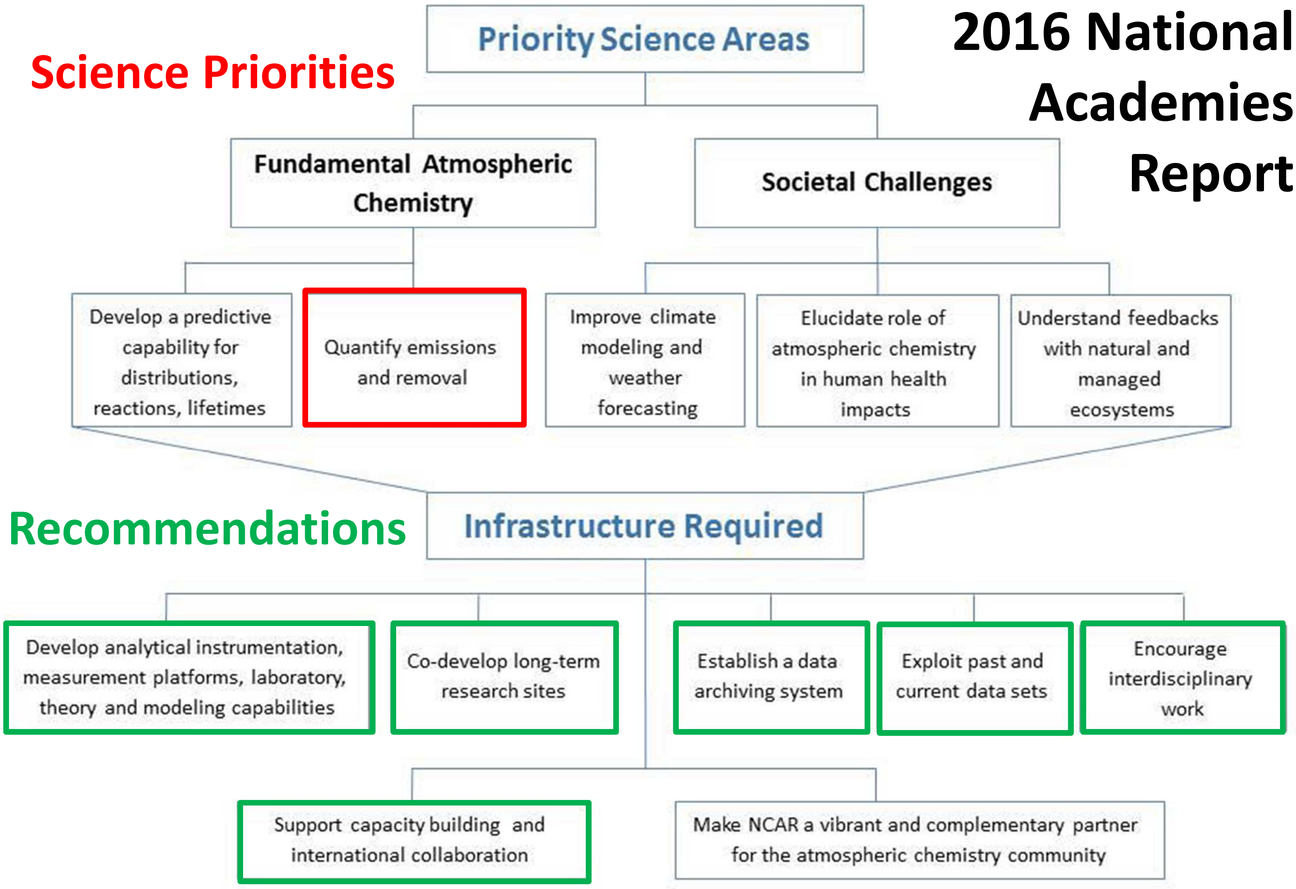
- Quantifiable uncertainties
- Quantify super-emitting or sporadic sources
- Detect cheating
- Complementary methods give confidence

Top-down methods complement bottom-up inventories, helping to improve the scientific basis of emissions.



We cannot manage what we can't measure – John Burrows

2016 National Academies Report



National Academies of Sciences, Engineering, and Medicine. 2016. The Future of Atmospheric Chemistry Research: Remembering Yesterday, Understanding Today, Anticipating Tomorrow.

Two Examples Today

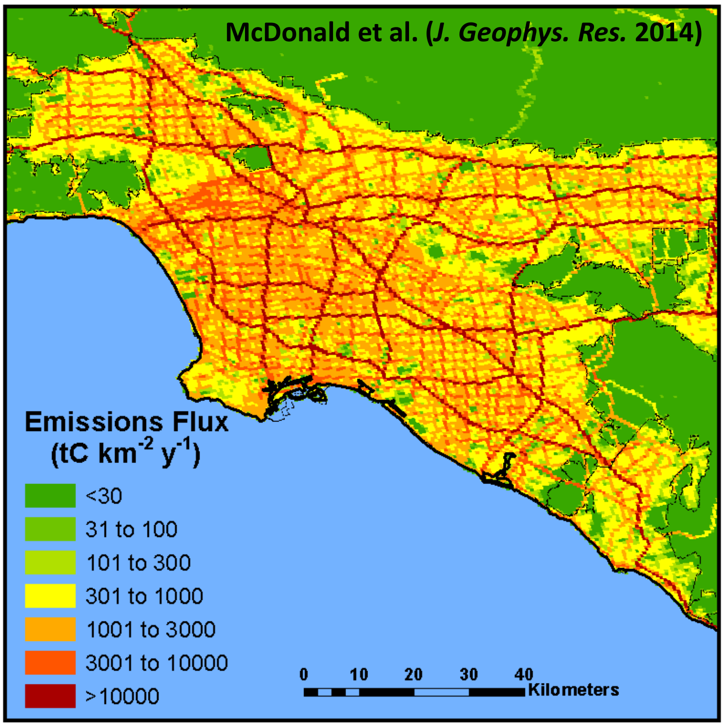
- US motor vehicles
- US oil and natural gas basins

Other NOAA examples I won't have time for:

- Power generation
- Refineries
- US vs European motor vehicles
- Well blowouts
- Agriculture
- Wildfires

Fuel-Based Inventory of Vehicle Emissions (FIVE)

Emissions = Activity (kg fuel) **x Emission Factor** (g/kg fuel)



Quantify on-road CO_2 emissions

- State-level taxable gasoline and diesel fuel sales reports
- Public and annual

Map on-road CO_2 emissions

- Using traffic count data
- Basis for scaling co-emitted combustion byproducts

Use of Roadway Studies for Emission Factors

Emissions = Activity (kg fuel) **x Emission Factor** (g/kg fuel)

Roadside monitoring data

- Measures in-use vehicles
- Captures high-emitters
- Regulatory models typically rely on chassis dynamometer tests

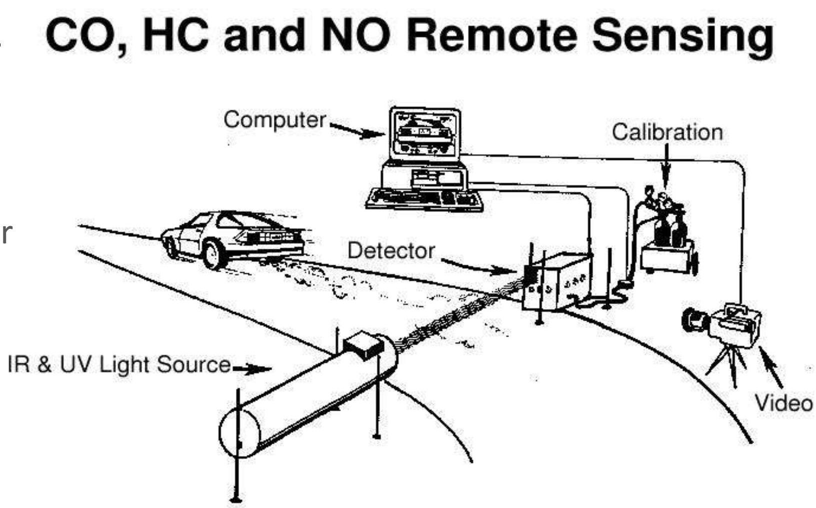
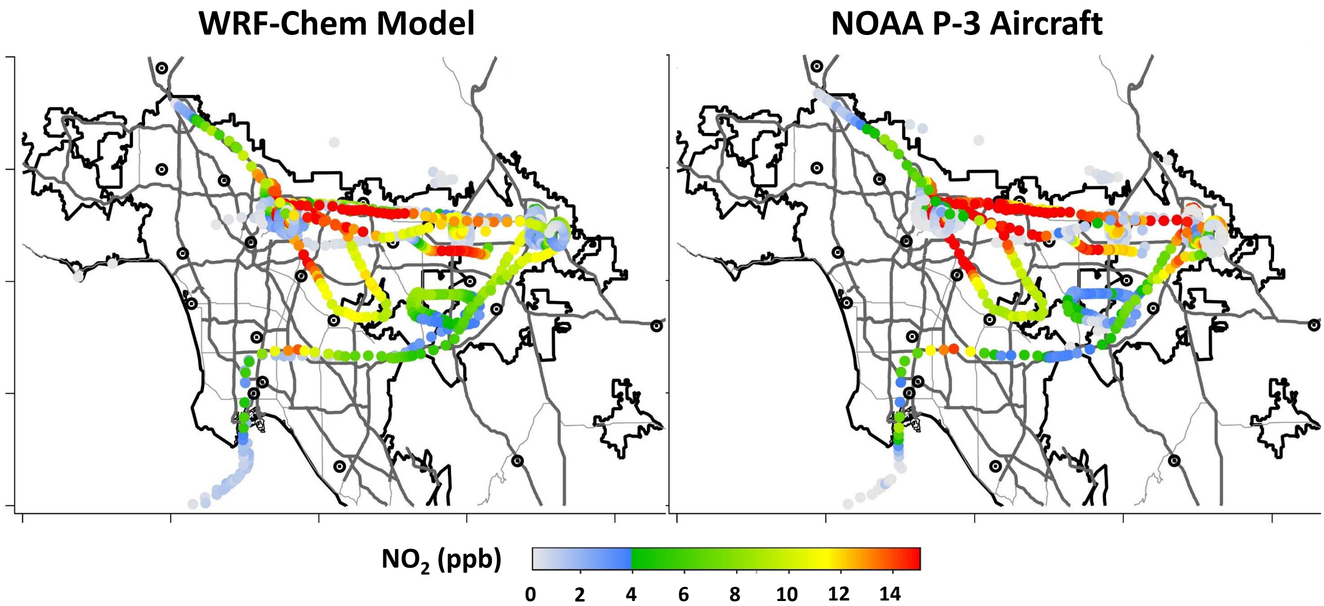


Figure from Univ. of Denver FEAT System

Test of Fuel-Based Emissions Approach



Simulated for California Nexus Study (CalNex) in 2010

- Los Angeles is good test case of transportation emissions (~2/3 of NO_x budget)

Si-Wan Kim et al. (*J. Geophys. Res.* 2016)

Long-Term Trends in U.S. On-Road NO_x Emission Factors

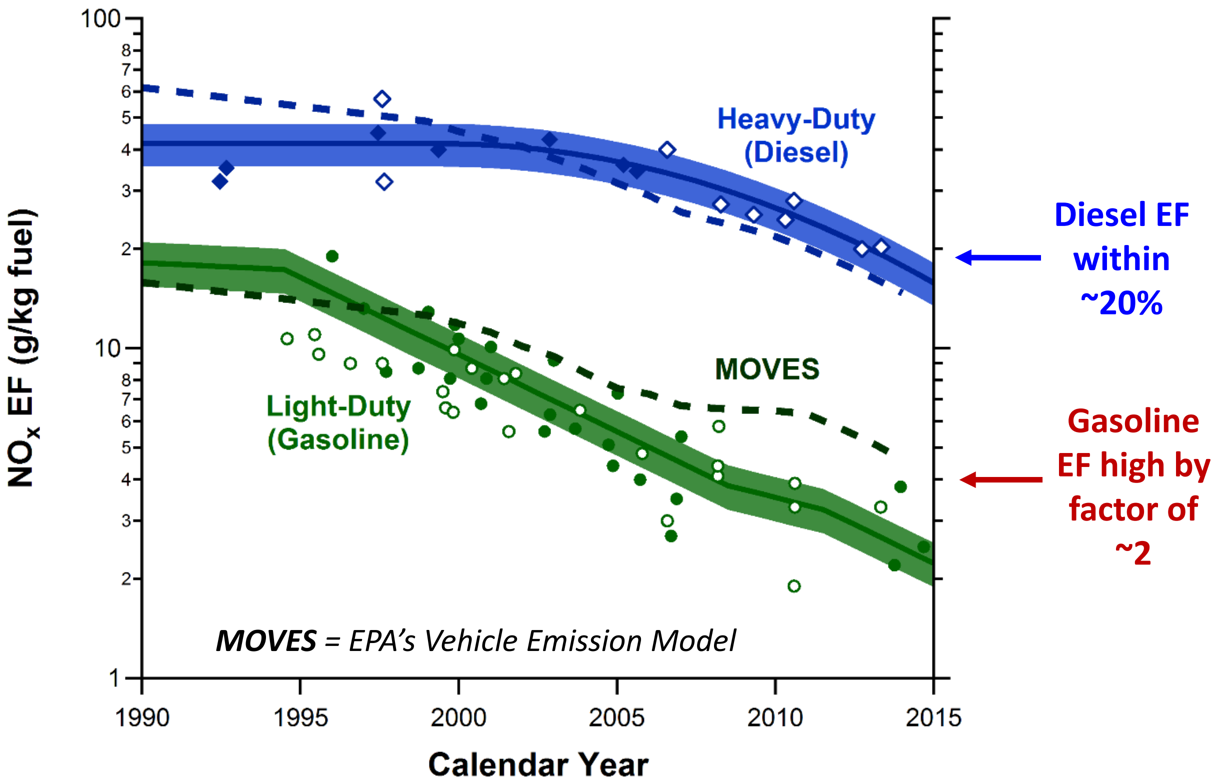
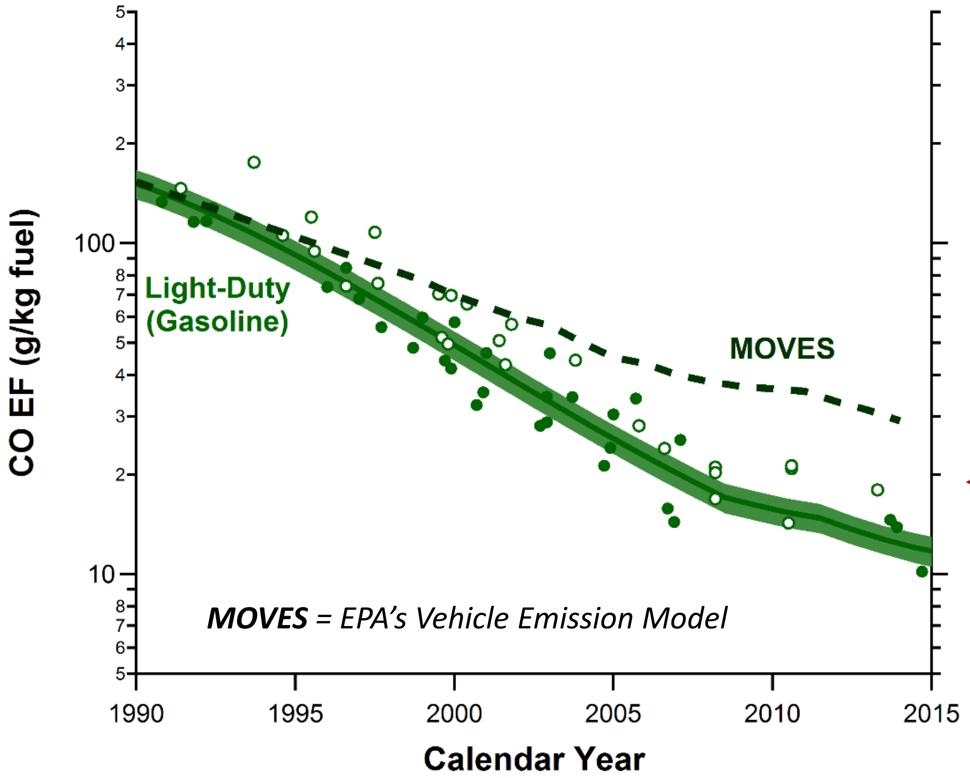


Figure updated from McDonald et al. (*J. Geophys. Res.* 2012)

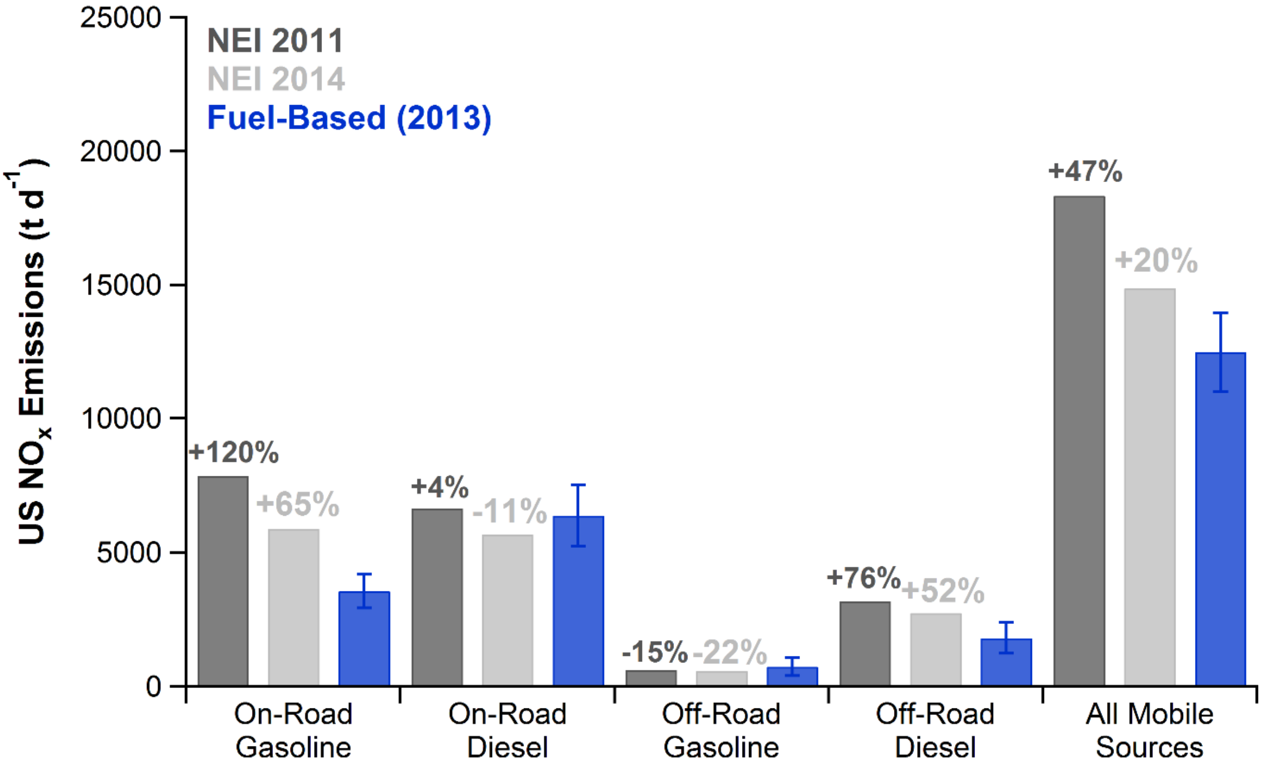
Long-Term Trends in U.S. On-Road CO Emission Factors



Gasoline EF high by factor of ~3

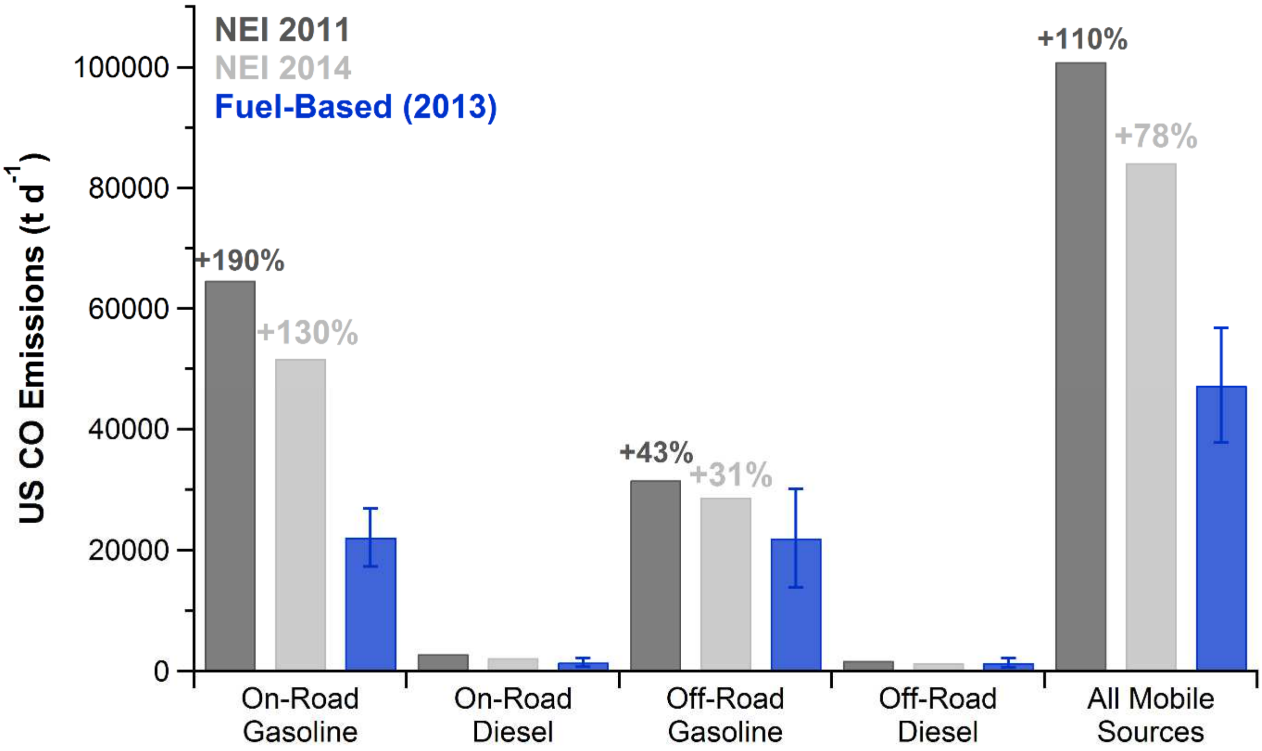
Figure updated from McDonald et al. (*Environ. Sci. Technol.*. 2013)

Comparing U.S. Mobile Source NO_x Emissions by Sector



McDonald et al. (*in preparation*)

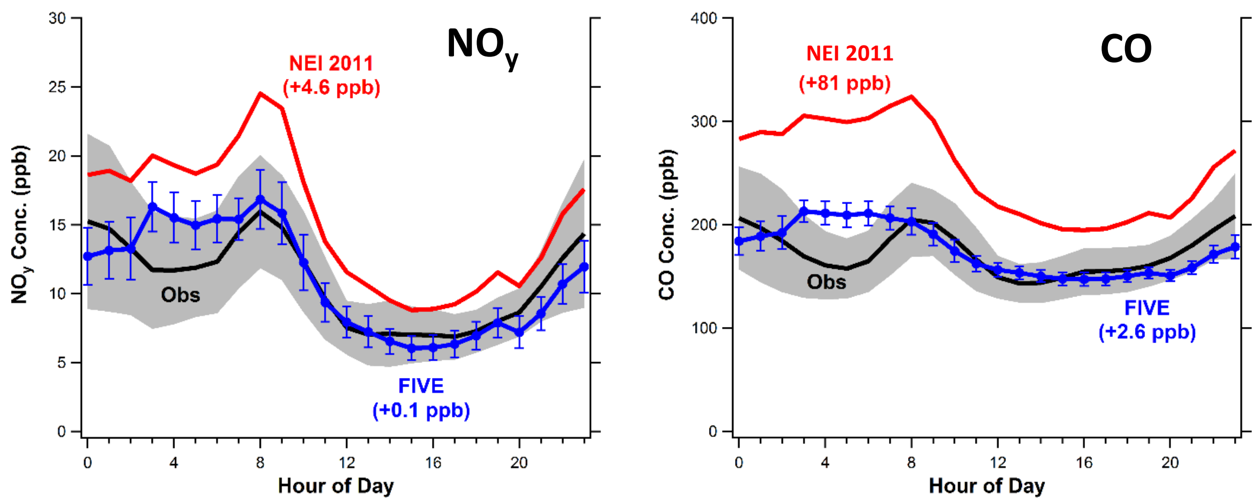
Comparing U.S. Mobile Source CO Emissions by Sector



McDonald et al. (*in preparation*)

Comparing Fuel-Based & NEI/MOVES in Regional Model

WRF-Chem modeling compared to summer 2013 observations at SEARCH network site in downtown Atlanta

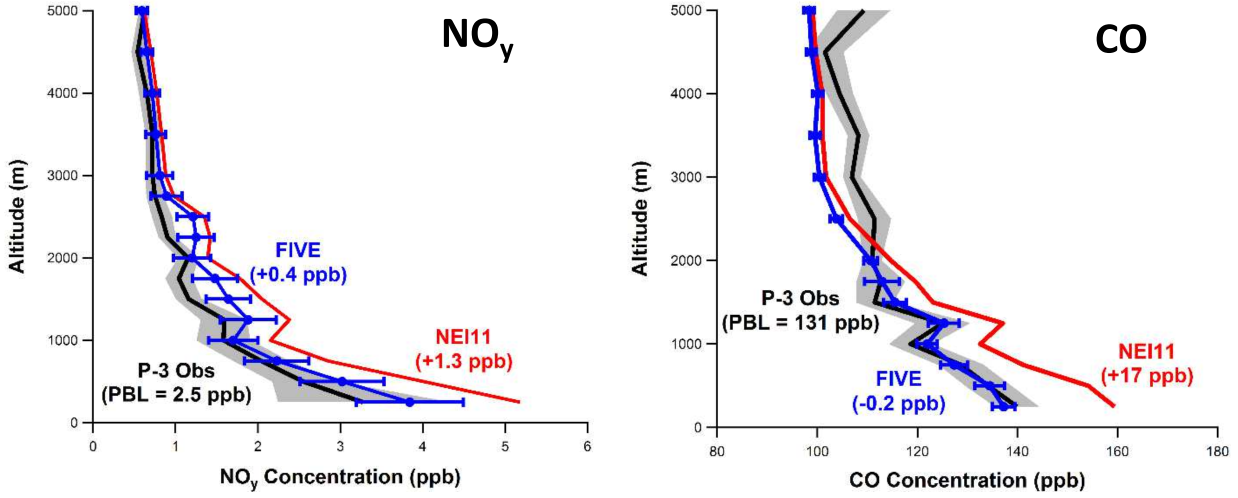


Model using fuel-based motor vehicle emissions captures ambient NOy and CO in urban areas better than EPA MOVES

McDonald et al. (*in preparation*)

Comparing Fuel-Based & NEI/MOVES in Regional Model

WRF-Chem modeling compared to vertical profile observations collected by the NOAA P-3 aircraft in Nashville in summer 2013



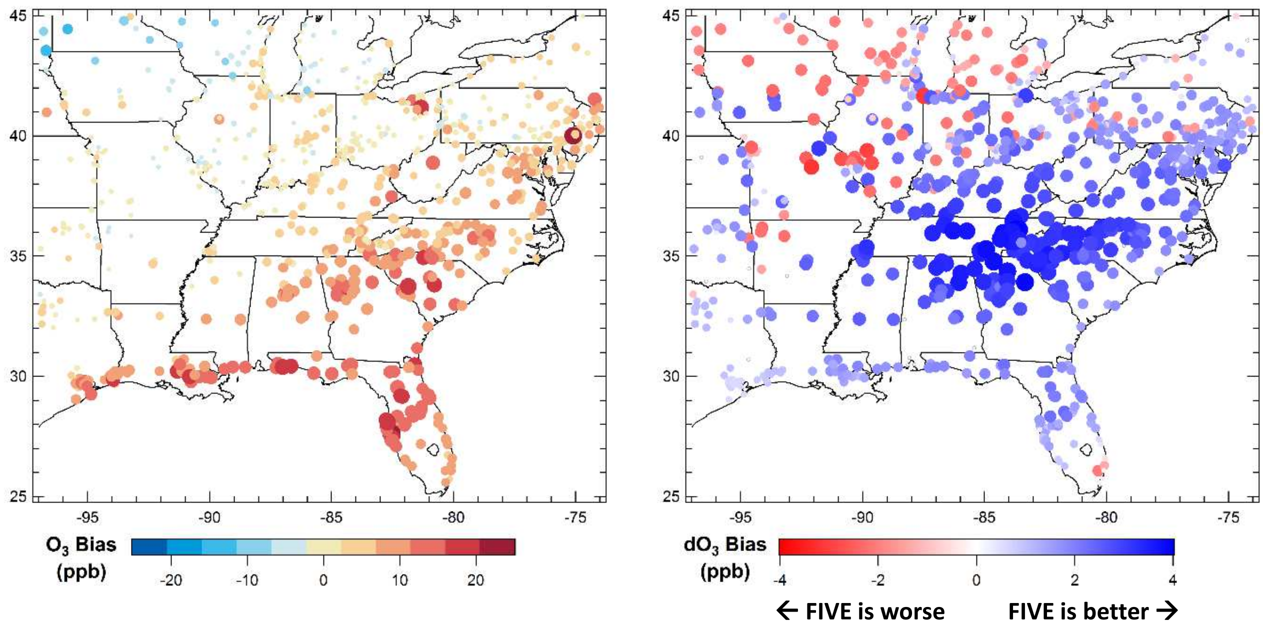
Model using fuel-based motor vehicle emissions captures ambient NOy and CO in urban areas better than EPA MOVES

McDonald et al. (*in preparation*)

Comparing Fuel-Based & NEI/MOVES in Regional Model

Mean bias (model-obs) in summer 2013 daily 8-hr O_3 max modeled with NEI 2011 vs. AQS data

Change in model-obs bias for daily 8-hr O_3 max (Δbias = |model(NEI 2011)-obs|-|model(FIVE) – obs|)

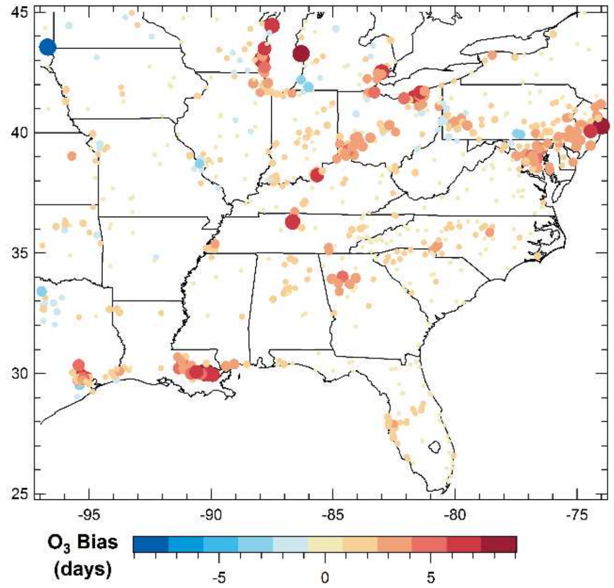


Model using fuel-based motor vehicle emissions captures regional maximum O_3 levels better than EPA MOVES

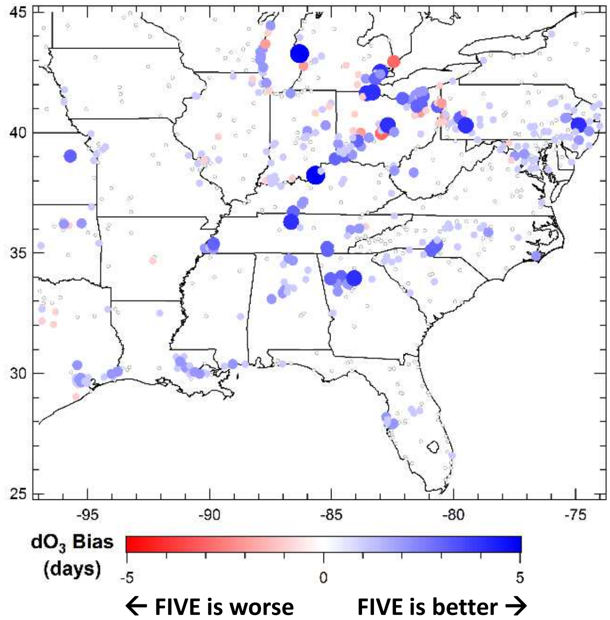
McDonald et al. (*in preparation*)

Comparing Fuel-Based & NEI/MOVES in Regional Model

Mean bias (model-obs) in 2013 O_3 exceedance days (>70 ppb) modeled with NEI 2011 vs. AQS data



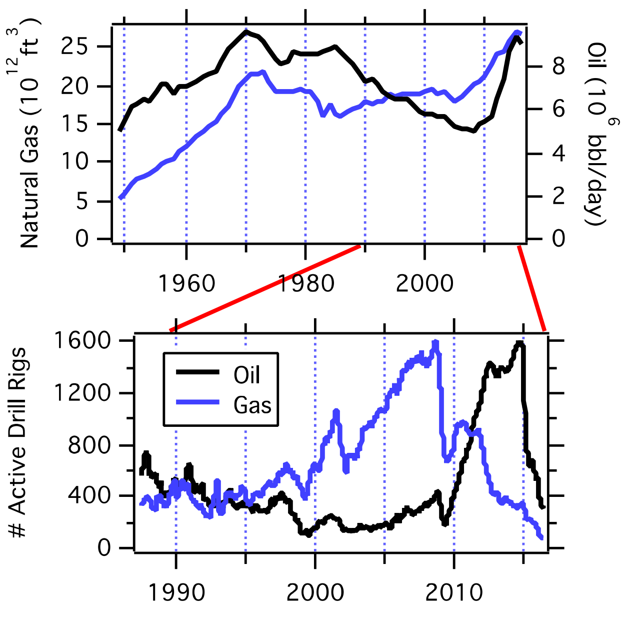
Change in model-obs bias for O_3 exceedance days (Δbias = |model(NEI 2011)-obs|-|model(FIVE) – obs|)



Model using fuel-based motor vehicle emissions captures regional O_3 exceedance days better than EPA MOVES

McDonald et al. (*in preparation*)

Quantifying Impacts of Oil and Gas Production



NOAA ESRL research is focused on:

A. Climate

Emissions of radiative forcing agents (methane, black carbon, CO_2, ozone)

B. Air quality

Emissions of ozone and PM2.5 precursors

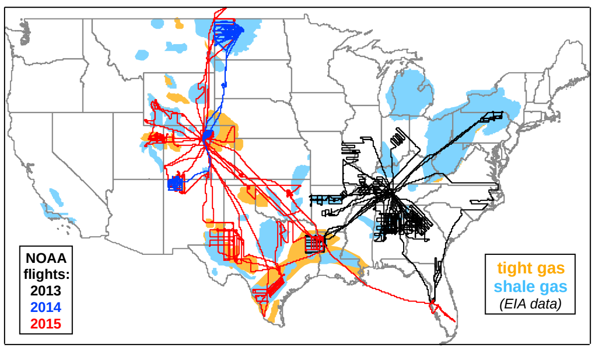
Understanding ozone formation

Emissions of air toxics (e.g. benzene)

ESRL research aircraft quantified methane (CH_4) emissions from regions accounting for

- **32%** of **U.S. oil production**
- **40%** of **U.S. natural gas production**
- **70%** of **U.S. shale gas production**

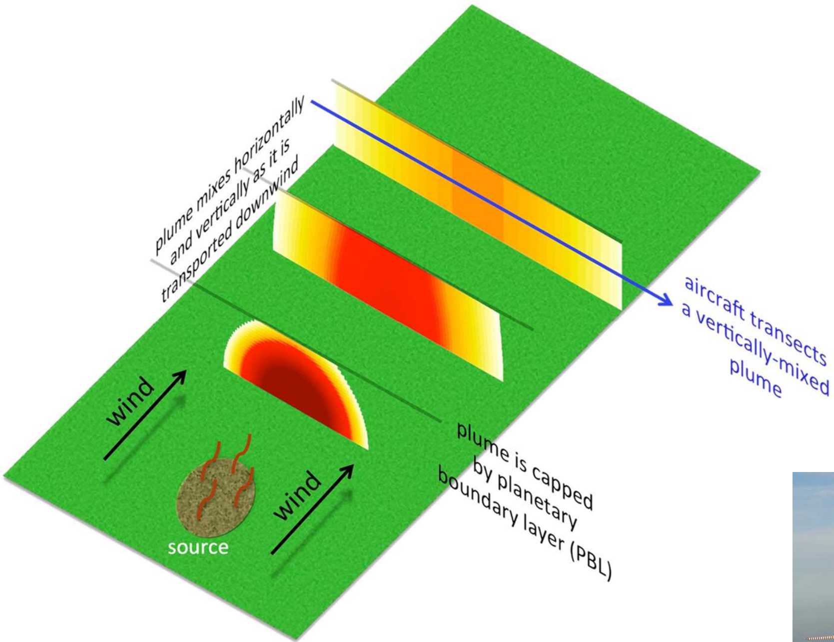
www.esrl.noaa.gov/csd/news/topics/oilandgas.html



Joost de Gouw

Mass balance flights directly measure CH_4 emissions rate

CH_4 emissions = (wind speed • mixing height • measured plume CH_4 enhancement)



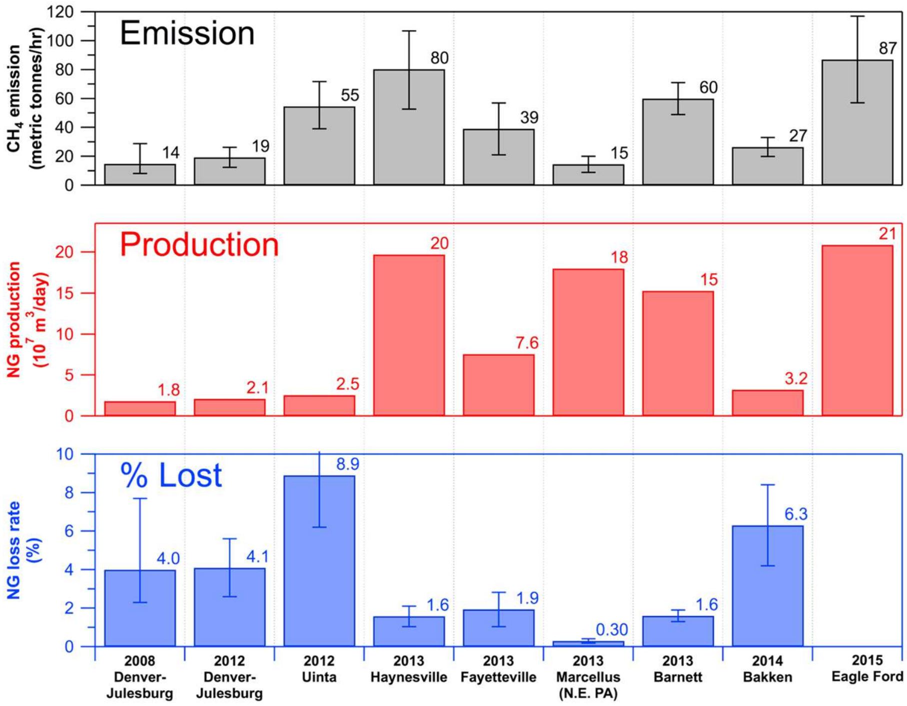
NOAA Twin Otter

Scientific Aviation Mooney

NOAA WP-3D

Jeff Peischl

Substantial regional variability in oil/gas CH_4 emissions

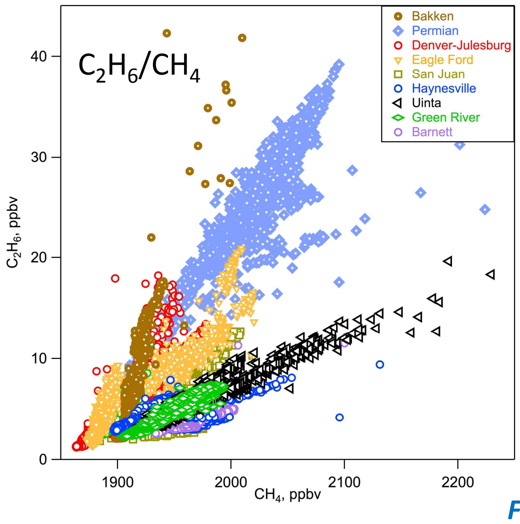


Regional emissions variability is high. Drivers include:
dry vs. wet gas formations, production activity, economic and regulatory framework

Interannual emissions variability appears low – at least on basin-wide scales.

Petron et al. JGR 2012; Petron et al. JGR 2014; Karion et al. GRL 2013; Peischl et al. JGR 2015; Peischl in prep

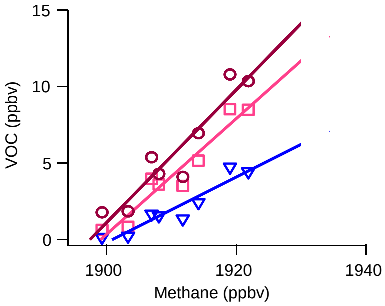
Using VOC/CH_4 Ratios to Quantify VOC Emissions



- VOCs and CH_4 are highly correlated with in a basin
- VOC/CH_4 enhancement ratios (ERs) provide a chemical fingerprint of oil/gas activity
- VOC/CH_4 ERs are basin specific

Flux(VOC) = Flux(CH_4) * ER(VOC/CH_4) * MW(VOC)/MW(CH_4)

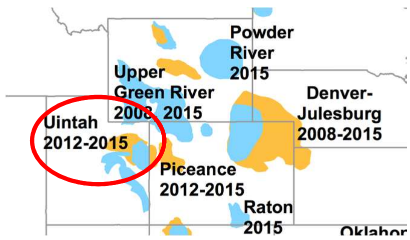
Combine CH_4 emissions derived from mass balance with VOC/CH_4 ERs to quantify emissions of different VOC species in a basin



VOC	$ER_{[VOC]/[CH4]}$	r	MW_{VOC}
Ethane	0.43 ± 0.06	0.94	30
Propane	0.38 ± 0.04	0.96	44
n-Butane	0.21 ± 0.03	0.94	58

Jessica Gilman, in preparation

Atmospheric Measurements Improve Oil/Gas Emissions in Uintah Basin



Emission datasets	Source	Methane (tons/year)	Non methane VOCs (tons/year)	NO_x (tons/year)
Bottom-up	EPA National Emission Inventory (NEI-2011)	100,279	101,184	16,448
Top-down	Based on the measurements	482,130	184,511	4,158

✓ Total top-down based methane flux estimate from *Karion et al., 2013*

✓ Total methane and other VOC emissions in NEI-2011 are lower by a factor of 4.8 and 1.8 than in the top-down estimates, respectively

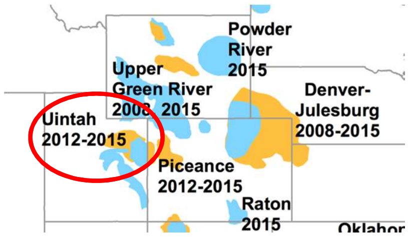
✓ Conversely, NO_x emissions are 4 times higher in the NEI-2011 inventory

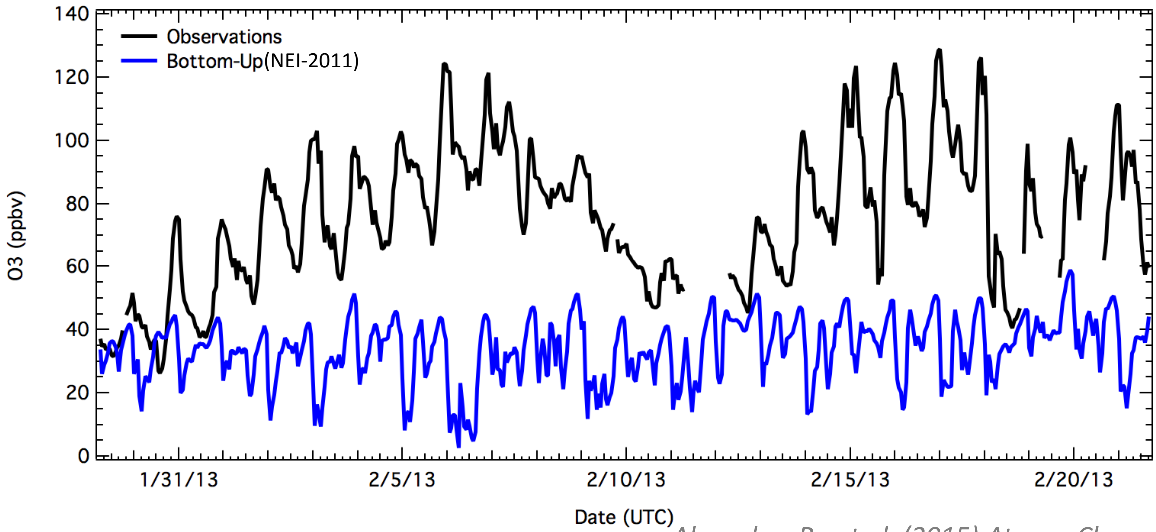
➢ Implications for air quality regulations and for climate and air quality impacts

Ahmadov, R., et al. (2015) Atmos. Chem. Phys.

Measurement-Based Emissions Improve WRF-Chem O_3 Predictions in Uintah Basin

- Multi-day buildup of surface O_3 during stagnation episodes
- Model using official bottom-up emissions inventory can't reproduce observed high O_3 levels

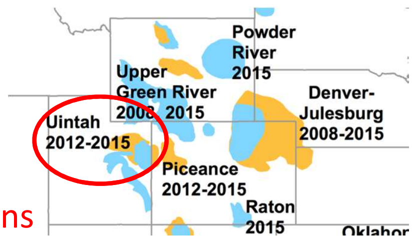


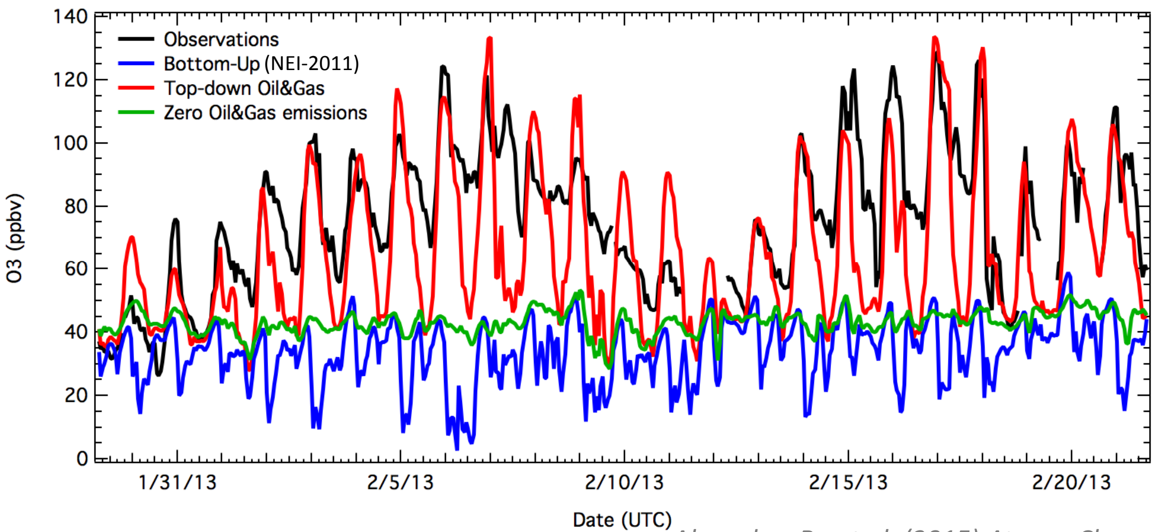


Ahmadov, R., et al. (2015) Atmos. Chem. Phys.

Measurement-Based Emissions Improve WRF-Chem O_3 Predictions in Uintah Basin

- Multi-day buildup of surface O_3 during stagnation episodes
- Model using official bottom-up emissions inventory can't reproduce observed high O_3 levels
- Measured emissions case explains high O_3 levels
- High O_3 in this basin driven mostly by oil/gas emissions





Ahmadov, R., et al. (2015) Atmos. Chem. Phys.

Better Collaboration Can Improve Inventories

Some examples:

- NOAA
- NASA
- AQRS
- GEIA

NOAA's Emissions Research Benefits Stakeholders

NOAA Stakeholders

ACADEMIA

What NOAA provides:

- Connect research to models
- Inform inventory development
- Synthesize information
- Nurture community of experts

Forms of outreach:

- Journal articles
- Conferences
- Assessments
- Direct outreach

NASA Air Quality Applied Sciences Team

Conveying NASA's science information to regulatory agencies

Primer on using satellites for emission estimates
by David G. Streets et al.

Atmos. Env., Vol. 77, October 2013, pp. 1011–1042

Atmospheric Environment 77 (2013) 1011–1042

Contents lists available at SciVerse ScienceDirect

Atmospheric Environment

journal homepage: www.elsevier.com/locate/atmosenv

ELSEVIER

ATMOSPHERIC ENVIRONMENT

Review

Emissions estimation from satellite retrievals: A review of current capability

CrossMark

David G. Streets[a,*], Timothy Canty[b], Gregory R. Carmichael[c], Benjamin de Foy[d], Russell R. Dickerson[b], Bryan N. Duncan[e], David P. Edwards[f], John A. Haynes[g], Daven K. Henze[h], Marc R. Houyoux[i], Daniel J. Jacob[j], Nickolay A. Krotkov[e], Lok N. Lamsal[e], Yang Liu[k], Zifeng Lu[a], Randall V. Martin[l], Gabriele G. Pfister[f], Robert W. Pinder[m], Ross J. Salawitch[b], Kevin J. Wecht[j]

NASA Training for the Bay Area Air Quality Management District

- September 10 - 12, 2013, Santa Clara, CA
- Hosted by BAAQMD
- 16 attendees from local AQ agencies, private sector, and academia
- **NASA aerosol products, and NASA / NOAA smoke/fire and products** and their applications to air quality monitoring.

Course Taught by Pawan Gupta and Yang Liu

1

NASA Air Quality Applied Sciences Team (AQAST)
10th Semiannual Meeting
EPA, Research Triangle Park
Jan 5-7, 2016

President Obama highlights value of satellite data for air quality analysis

aqast.org

Federal Interagency Cooperation on Air Quality

Office of Science and Technology Policy's National Science and Technology Council

Committee on Environment, Natural Resources, and Sustainability (CENRS)

Air Quality Research Subcommittee (AQRS)

Co-chairs:

Dan Costa National Program Director, ORD's Air, Climate, and Energy Research Program
John Daniel Deputy Director, Chemical Sciences Division, NOAA Earth System Research Lab

Goals: To enhance the effectiveness and productivity of U.S. air quality research and to improve information exchange on air quality issues, including the scientific knowledge base for air quality standards and compliance assessment.

Ongoing topics of interagency discussion and coordination:

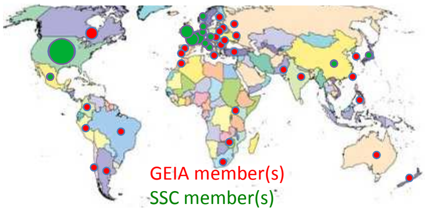
- Ozone transport (tropospheric and stratospheric) and the NAAQS
- Wildfires: Future field experiments to improve understanding of emissions, chemical transformations, transport, and impacts
- Appropriate response to the report by the National Academies of Sciences, Engineering, and Medicine on the future of atmospheric chemistry research

International Emissions Efforts

GEIA Global Emissions InitiAtive

Community
Strengthening the emissions community by connecting developers and users

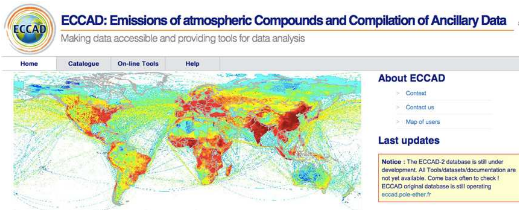
2000 people worldwide

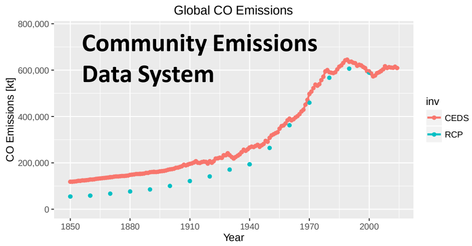


www.geiacenter.org

IGAC ileaps AIMES

Access
Creating easier, more open access to emissions data and information





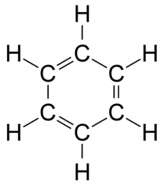
www.globalchange.umd.edu/ceds/

Analysis
Identifying priorities, facilitating research, and synthesizing findings to improve the scientific basis of emissions

China Working Group

Latin America/ Caribbean WG

VOC WG



Assessing Emissions Quantification using Inverse Modeling (joint with IGAC)

Some Final Thoughts

- Emissions are critical to decision making
- Inventories are fundamental datasets with many challenges
- Atmospheric observations and models complement inventories and help inform emissions understanding
- Reconciling approaches improves scientific basis
- Structures exist to work together nationally and globally
- Guiding principles:
  - Humility
  - Flexibility
  - Communication
  - Collaboration

附錄五　**Advances in meteorological modeling and data assimilation**

Advances in Meteorological Modeling and Data Assimilation

15th CMAS Conference
Plenary Session
"Emerging Issues in Air Quality Modeling"

Chapel Hill, NC
24 October 2016

David R. Stauffer
Penn State University

OUTLINE

- Overview of US global model cores for Next Generation Global Prediction System (NGGPS) – first step toward model unification across scales?

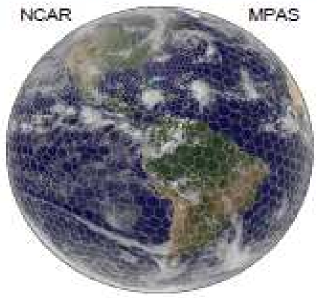
- Advances in model physics, with focus on surface layer and SBL

- Use of ensembles for quantifying uncertainty

- Controlling noise / "seams" in driver MET data, effective use of advanced intermittent data assimilation (e.g., EnKF), hybrid methods!

- Recommendations

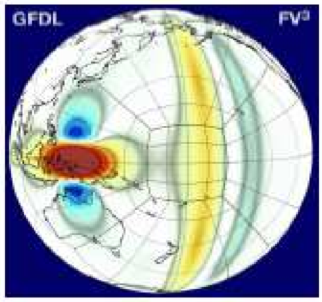
Next Generation Global Prediction System (NGGPS)



Phase 2 Atmospheric Dynamic Core Evaluation

Presentation
For UMAC

Fred Toepfer/Tim Schneider, Program Manager
Dynamic Core Test Group
June 22, 2016



New Dynamic Core Candidate Models

Phase 1 Testing Included*:

*Built upon HIWPP Non-hydrostatic Model Evaluation

- Non-hydrostatic Global Spectral Model (GSM) - EMC
- Global Non-hydrostatic Mesoscale Model (NMM & NMM-UJ) - EMC
- → Model for Prediction Across Scales (MPAS) - NCAR
- Non-hydrostatic Icosahedral Model (NIM) – ESRL
- Navy Environmental Prediction System Using the NUMA Core (NEPTUNE) – Navy
- → Finite Volume Model version 3 – (FV3) – GFDL

- **FV3 and MPAS selected to advance to Phase 2**

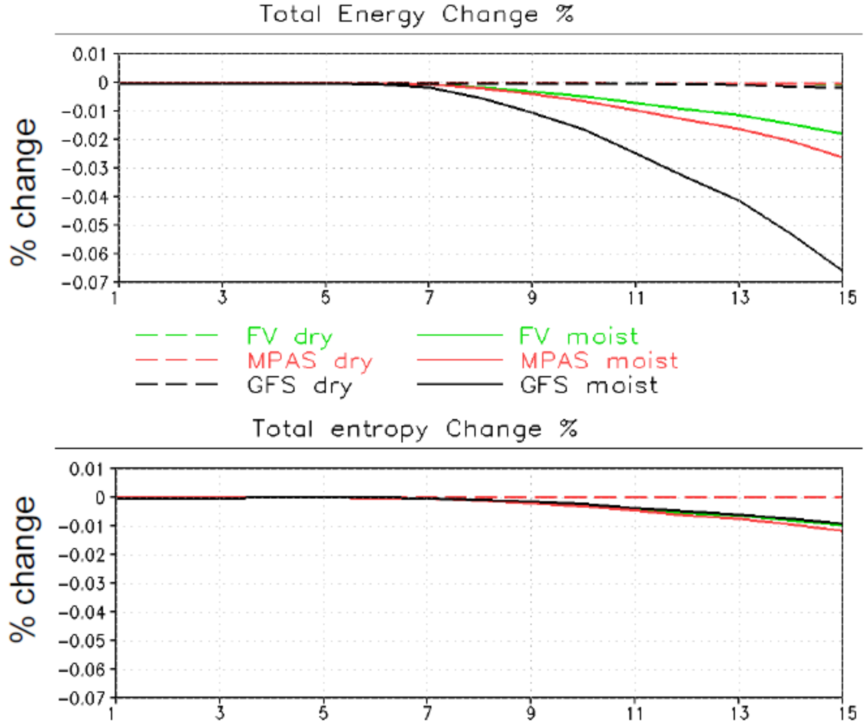
#2: Conservation Tests
Change in Total Energy and Entropy

Change in total energy (top) and entropy (bottom) as a percent change from the initial value. ***Note very tiny range on y axis.***

Energy loss nearly zero in dry case, FV3 and MPAS lose less energy than GFS in moist case.

Energy loss in moist case for FV3 and MPAS is consistent with the energy removed along with condensate. Entropy changes for moist case are very small, and consistent with thermodynamic approximations made in entropy definition.

Dry mass (not shown) is conserved exactly in both FV3 and MPAS, GFS gains 0.05 hPa during integration.



Summary of Phase 2 Test Results

- Testing yielded sufficient information to evaluate both dynamic cores and produce a low risk recommendation without compromising performance or skill
- Summary of results:
  - Computationally, FV3 is more than twice as fast as MPAS with equivalent resolution
  - FV3 performs comparable to the GFS in cycled data assimilation test (without tuning, at reduced resolution), MPAS performance inferior to GFS
  - → Effective resolution for both dynamic cores is found to be similar, and higher than GFS
  - Full forecast experiments with GFS initial conditions and GFS physics showed significant differences between FV3 and MPAS, FV3 almost equivalent to GFS (some stability issues with MPAS forecasts)
  - → Supercell tests showed subjectively similar results for both dynamic cores
  - MPAS has unresolved issues in TC and conservation tests

(NCAR ceased participation and withdrew from Dycore Test Group on 20 May 2016)

Summary and Conclusions

- The FV3 Core represents the lowest risk, lowest cost alternative for the new NGGPS atmospheric model
- Adopting FV3 core brings with it a dynamic, vibrant community
  - GFDL is a world-class organization in Global Modeling Applications for Weather and Climate
  - GFDL is a willing partner to the NWS in advancing operational Global weather modeling applications
  - Other Agencies/Entities using Finite Volume Core include NCAR (CESM), NASA (GEOS/GISS), Harvard (GEOS-Chem), Columbia Univ. (pollution studies), U. of Washington (Dale Durran), Chinese Academy of Sciences (IAP), Germany (ECHAM5), Japan (MIROC)
- Integration of FV3 with Common Community Physics Package and GMTB can support interaction with convective weather modeling community
- From the beginning, the NGGPS strategy has been to find and implement the best global model (unification at regional scales/picking the best convective model, while desirable, has not been an objective of NGGPS)
  - Nothing in results precludes eventual global-regional unification based on FV3

NGGPS Global Atmospheric Prediction Model Implementation Strategy

- Phase 1 – Identify Qualified Dynamic Cores
  - Evaluate technical performance
    - Scalability
    - Integration of scheme stability and characteristics
- Phase 2 – Select Candidate Dynamic Core
  - Integrate with operational GFS Physics/CCPP
  - Evaluate meteorological performance
- Phase 3 – Operational Implementation
  - Implement candidate dynamic core in NEMS
  - Implement Common Community Physics Package
  - Implement data assimilation (4DEnVar with 4D incremental analysis update and stochastic physics)

MPAS
Model for Prediction Across Scales

MPAS Home

Overview

MPAS-Atmosphere
MPAS-Land Ice
MPAS-Ocean
MPAS-Seaice
Data Assimilation
Publications ←
Presentations ←

Download

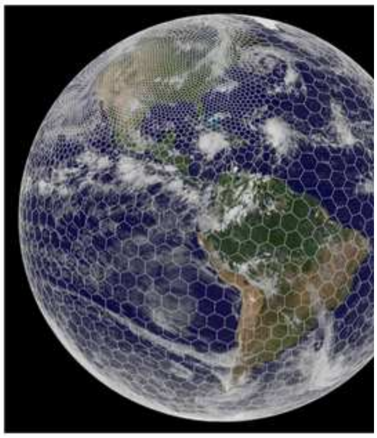
MPAS-Atmosphere download
MPAS-Land Ice download
MPAS-Ocean download

Resources

License Information
Wiki
Bug Tracker
Mailing Lists
MPAS Developers Guide ←
MPAS Mesh Specification Document

MPAS Overview

The Model for Prediction Across Scales (MPAS) is a collaborative project for developing atmosphere, ocean and other earth-system simulation components for use in climate, regional climate and weather studies. The primary development partners are the climate modeling group at Los Alamos National Laboratory (COSIM) and the National Center for Atmospheric Research. Both primary partners are responsible for the MPAS framework, operators and tools common to the applications; LANL has primary responsibility for the ocean and land ice models, and NCAR has primary responsibility for the atmospheric model.

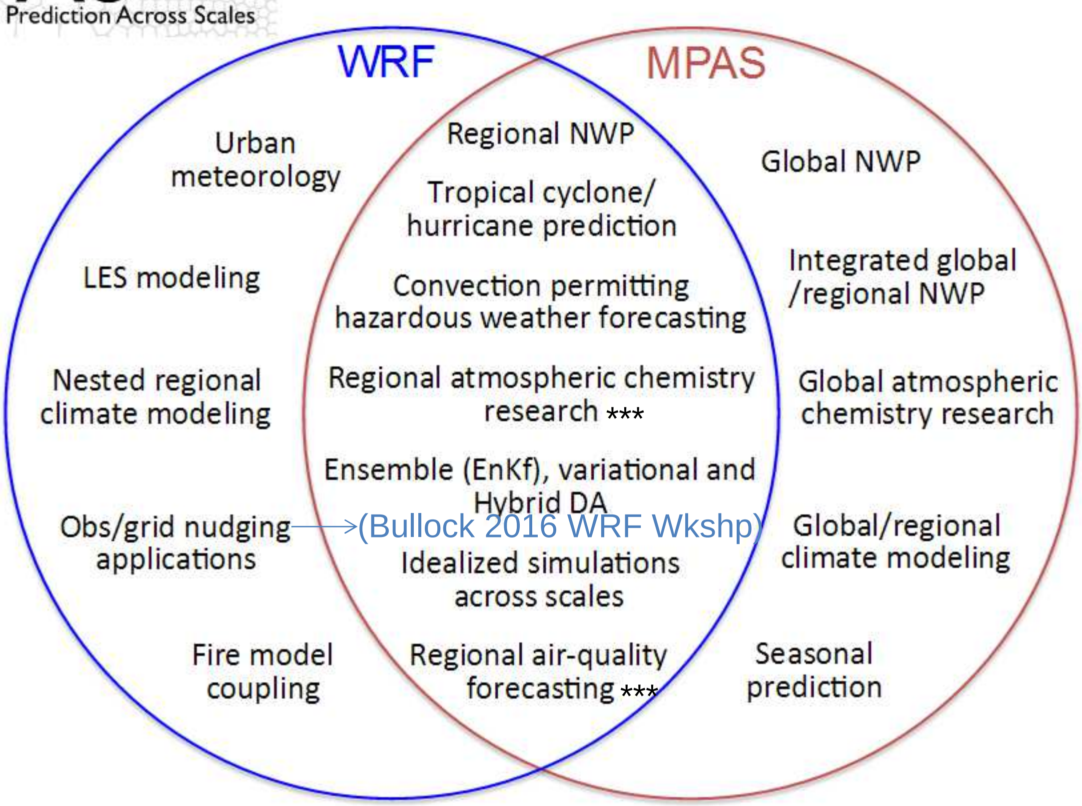


The defining features of MPAS are the unstructured Voronoi meshes and C-grid discretization used as the basis for many of the model components. The unstructure Voronoi meshes, formally Spherical Centriodal Voronoi Tesselations (SCVTs), allow f both quasi-uniform discretization of the sphere and local refinement. The C-grid discretization, where the normal component of velocity on cell edges is prognosed, i especially well-suited for higher-resolution, mesoscale atmosphere and ocean simulations. The land ice model takes advantage of the SCVT-dual mesh, which is a triangular Delaunay tessellation appropriate for use with Finite-Element-based discretizations.

The current MPAS release is version 4.0. Please refer to each core for changes, and t github repository for source.

MPAS
Model for Prediction Across Scales

MPAS and WRF Applications



MPAS is not intended to replace WRF! Regional MPAS… ?

PENNSTATE 1855

Model Physics Advancements

PENNSTATE 1855

Jiminez et al. 2016a (BAMS)

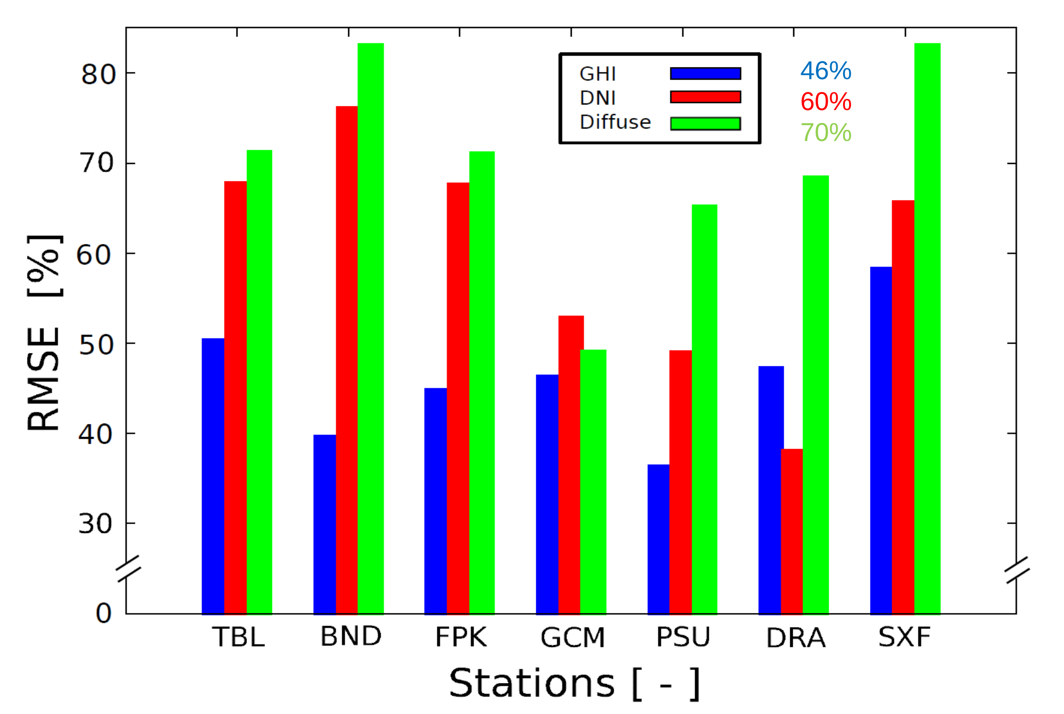
TABLE 1. Comparison of WRF and WRF-Solar developments.

	WRF-Solar	WRF
Solar energy applications	Output DNI and DIF	—
	High-frequency output of surface irradiance	—
	Solar position algorithm includes EOT	EOT is not included
Aerosol–radiation feedbacks	Observed/model climatologies or time-varying aerosols	Model climatology
Cloud–aerosol feedbacks	Aerosol indirect effect represented	—
Cloud–radiation feedbacks	Cloud particles consistent in radiation and microphysics	—
	Shallow cumulus feedback to radiation	—
	Fully coupled aerosol–cloud–radiation system	Uncoupled

1250 | BAMS JULY 2016

WRF-Solar code is OpenSource – some in general WRF release, and all in open wiki: https://wiki.ucar.edu/display/Sun4Cast/Sun4Cast+Home.

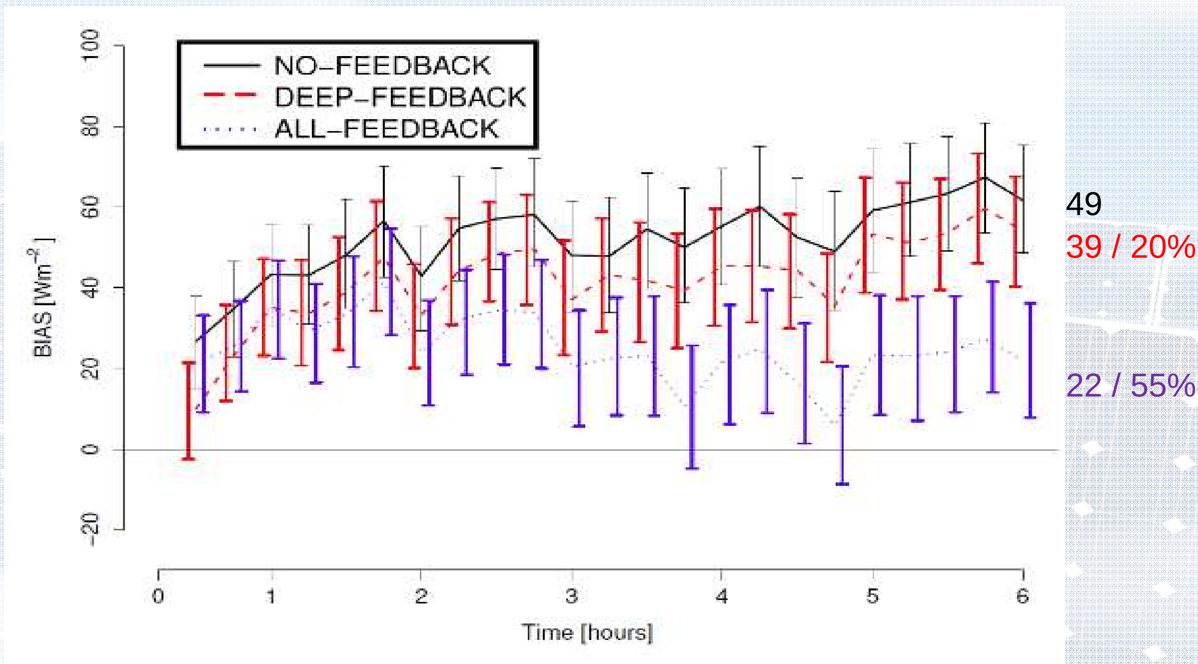
WRF-Solar *versus* Standard WRF Clear sky



Jiminez et al. 2016a (BAMS)

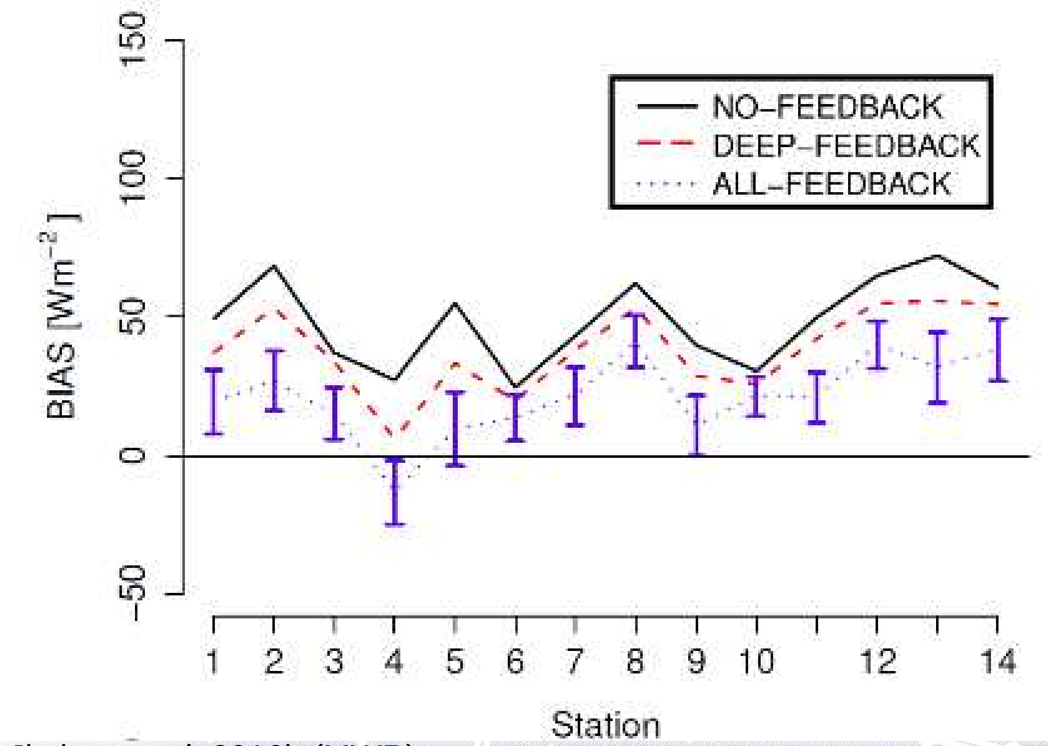
Results: unresolved-cloud model biases (1/3)

Standard WRF has a positive bias in GHI
Bias largely suppressed when the effects of unresolved clouds are activated



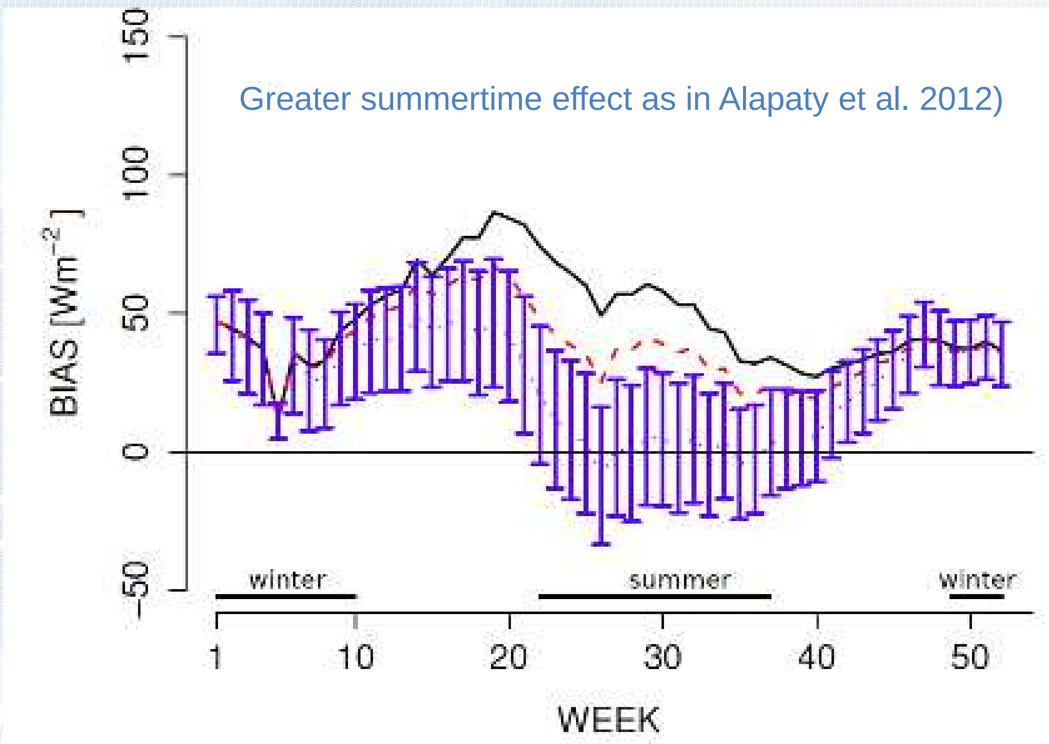
Jiminez et al. 2016b (MWR)

Results: unresolved-cloud model biases (2/3)



Jiminez et al. 2016b (MWR)

Results: unresolved-cloud model biases (3/3)



Jiminez et al. 2016b (MWR)

FASDAS:

Flux-Adjusting Surface Data ssimilation System (Alapaty et al., 2008)

FASDAS has two components:

- **DIRECT nudging of surface air (T_1 and Q_1)**
- **INDIRECT nudging of soil (T_g and Q_{soil})**

(Alapaty et al. 2016 WRF Users' Workshop)

FASDAS…

$$H_S^F = \rho C_p (\partial \theta_1^F / \partial t) \Delta z / \hat{E}$$

$$H_\ell^F = \rho L (\partial q_1^F / \partial t) \Delta z$$

$H_s^F = Adjustment\ Sensible\ Heat\ Flux$ ←

$H_\ell^F = Adjustment\ Latent\ Heat\ Flux$ ←

We use H_s^F and H_ℓ^F to adjust:

- soil moisture and
- soil temperature.

The updated ground/skin temperature can be written as:

$$T_g^F = T_g^n \frac{1}{C_g} \left(H_S^F - \psi_q H_\ell^F \right) \Delta t$$

SUMMARY

Flux-Adjusting Surface Data Assimilation System

- Avoids tuning coefficients by using boundary layer process knowledge
- Tested across *all* spatial scales
- Functional in summer or winter, day or night
  - → Need high-resolution reanalysis (4, 1 km grids) ←
- Generic for implementation into any LSM in regional and global models
- Improved meteorological inputs should help produce better environmental modeling ←

Stauffer 2012, Ch. 29, Uncertainty in Environmental NWP Models, Handbook of Environmental Fluid Dynamics, CRC Press, H.J.S. Fernando, Ed.

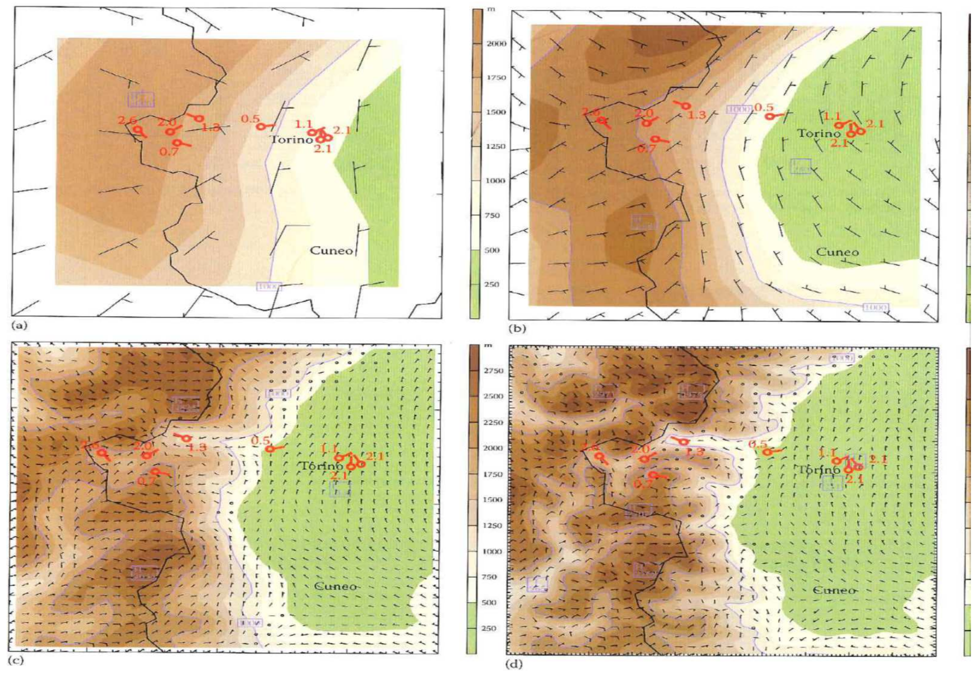
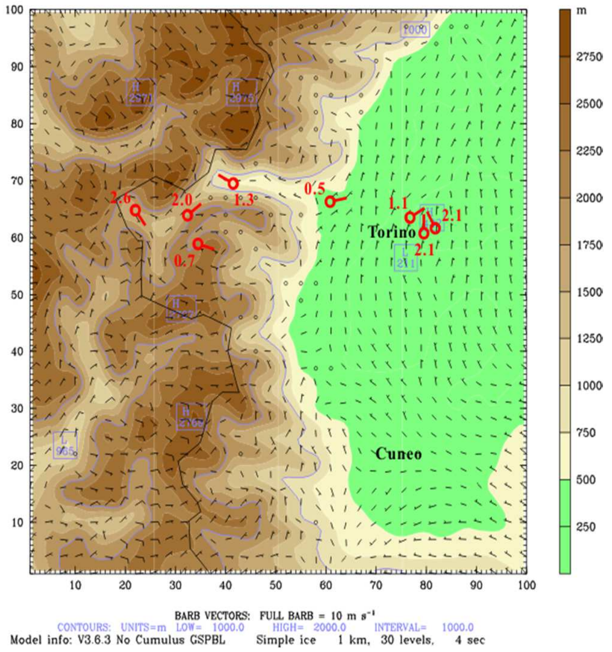


FIGURE 29.2 Sample MM5 NWP model surface wind prediction and special mesonet observations at 18 UTC February 21, 2006, over 1.3-km Torino Winter Olympics domain area for each model resolution forecast. Surface winds (m s^{-1}) are overlaid on the terrain field (m, c code on right of figure) for each model resolution domain. (a) 36-km domain, (b) 12-km domain, (c) 4-km domain, and (d) 1.3-km domain. full barb is 10 m s^{-1}. Dark line is France-Italy border. (After Stauffer, D.R. et al., On the role of atmospheric data assimilation and model resolu on model forecast accuracy for the Torino Winter Olympics, 11A.6, *22nd Conference on Weather Analysis and Forecasting/18th Conferenc Numerical Weather Prediction*, Park City, UT, June 25–29, 2007b, available at http://ams.confex.com/ams/pdfpapers/124791.pdf).

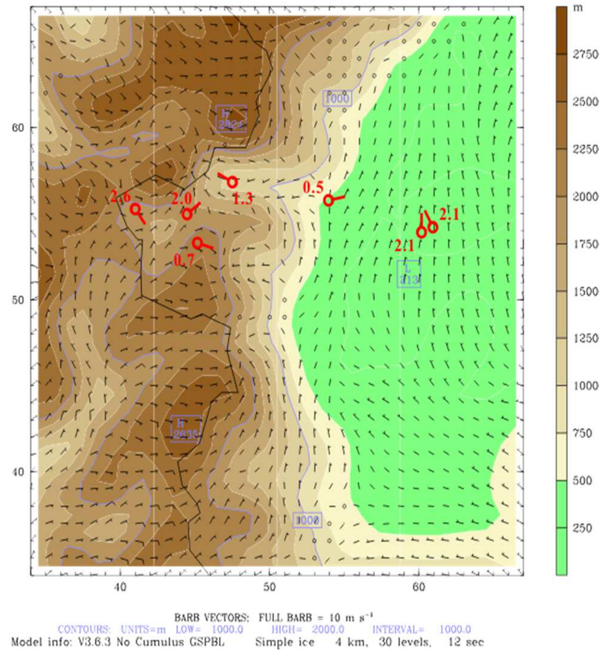
PENNSTATE 1855

Obs nudging for fine-resolution complex terrain….

1.3-km domain



4-km domain



PENNSTATE 1855

Stauffer and Seaman 1994, MWR

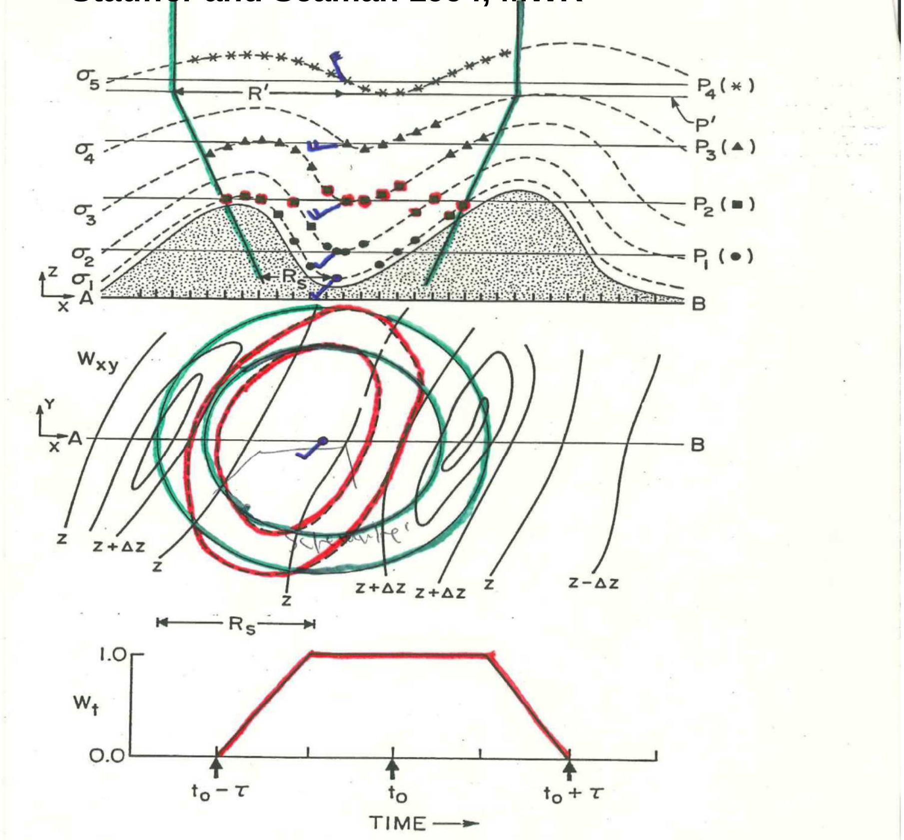


Figure 3. Schematic showing the horizontal weighting function, w_{xy}, and the temporal weighting function, w_t, used for obs nudging. Refer to text in section 2b for details.

附錄六　**A new version of the Community Multiscale Air Quality Model: CMAQv5.2**

EPA

CMAQv5.2 and Next Generation AQ Model

Jonathan Pleim and the CMAQ Development Team

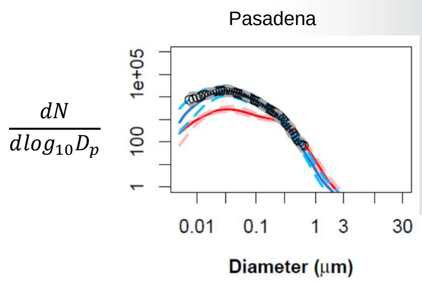
Atmospheric Model Development Branch
Computational Exposure Division
National Exposure Research Laboratory
Office of Research and Development
U.S. Environmental Protection Agency

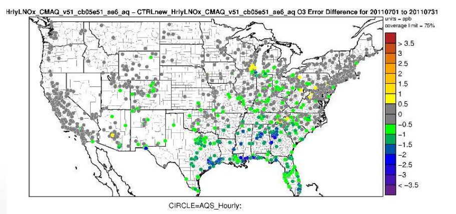
CMAS Conference
October 24, 2016

EPA

CMAQv5.2

- **Release schedule**
  - β-version released in October 2016: https://github.com/USEPA/CMAQ
  - Final version in Spring 2017
- **New features**
  - Aerosols
    - New SOA modeling (Talks by Havala Pye and Ben Murphy today)
    - New wind-blown dust model (Talk by Hosein Foroutan this morning)
    - New particle formation in research version (Ben Murphy poster)
  - Gas Chemistry
    - CB6 chemical mechanism w/ selected HAPs
    - CRI mechanism in research version (Deborah Luecken)
    - Halogen Chemistry (Golam Sarwar poster)
      - Optional detailed mechanism (Sarwar et al., ES&T, 2015)
  - Lightning
    - NOx production (Talk by Daiwen Kang this morning)
    - Assimilation of lightning data in WRF (Talk by Nick Heath - Wed)
  - Instrumented models – DDM, Sulfur tracking (in final model)
  - Strat-Trop ozone exchange for hemispheric configuration
  - 2-way coupled WRFv3.8-CMAQv5.2

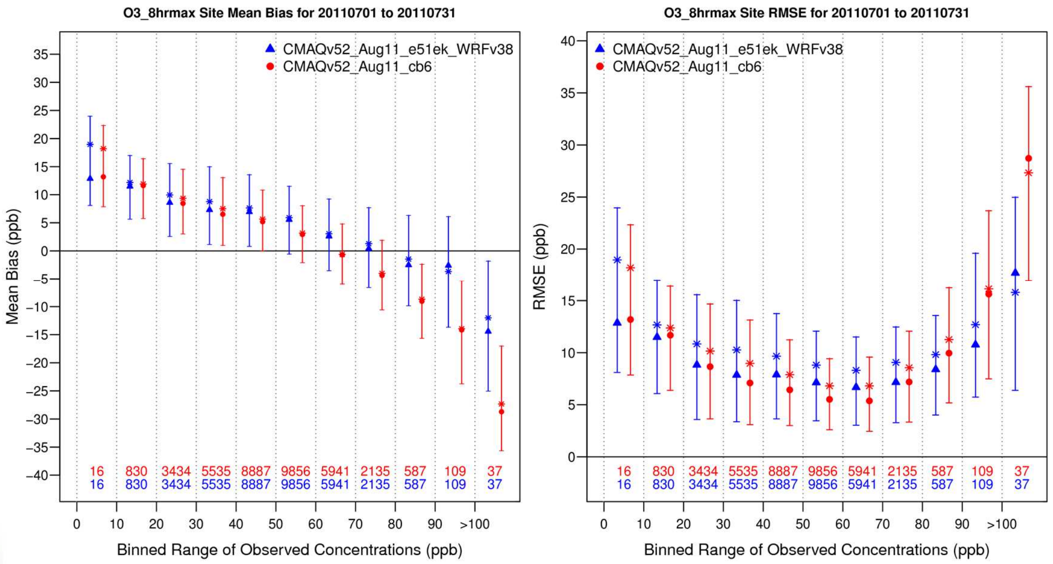




O_3 MAE improvement w/ LTGA

Gas-phase chemistry

Comparison of predicted Ozone in CMAQv5.2 with two mechanisms (CB05e51 and CB6r3)



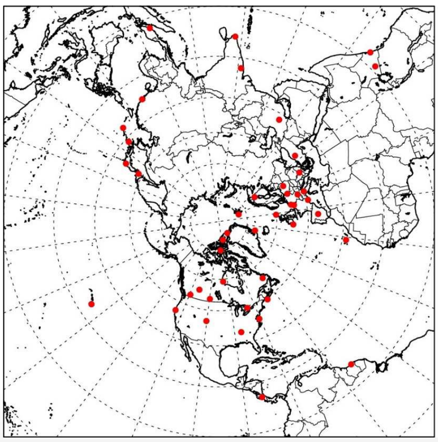
CB6 predicts slightly lower ozone, with lower bias and error below ~80 ppb, increased bias and error above 80 ppb.

Courtesy of Deborah Luecken

CMAQv5.2 Updates:
Stratosphere-Troposphere Exchange

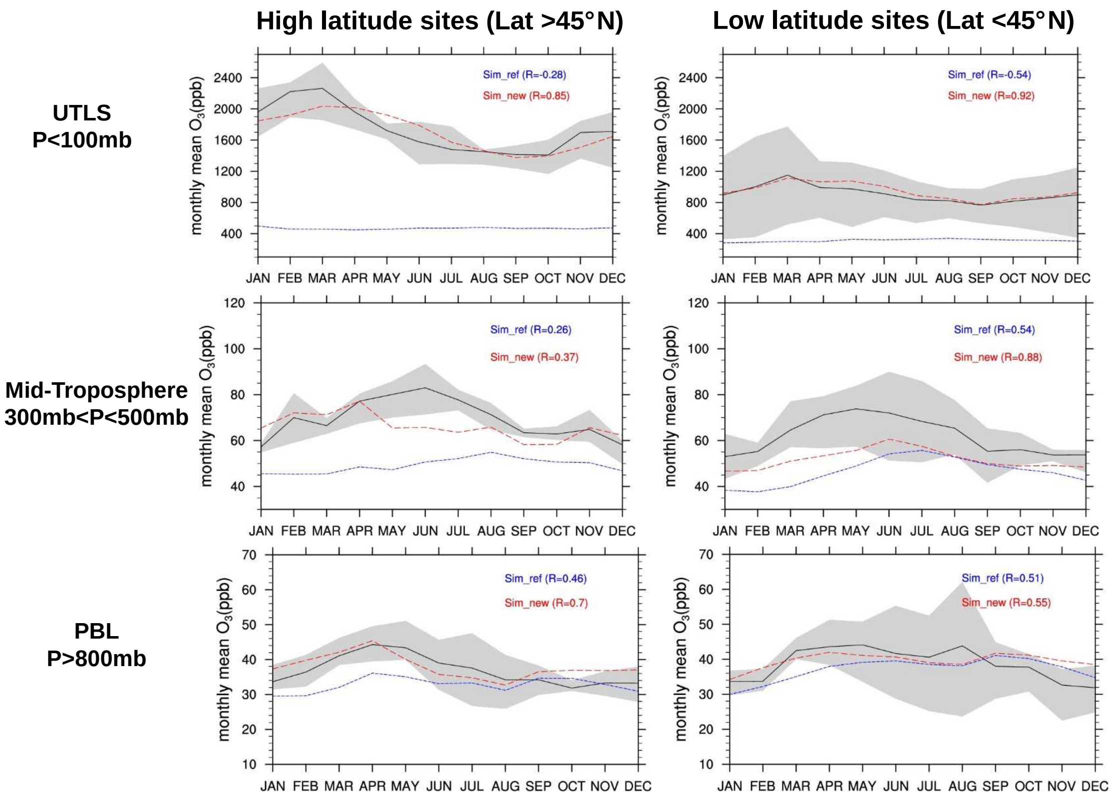
- Modeled O_3 specified by enforcing the condition of proportionality to Potential Vorticity: ***$[O_3]$ = c•PV***
- Used recent CMAQ multi-decadal simulations to develop a robust relationship that varies spatially and temporally: O_3/PV = F(*spatial*) X G(*temporal*)

Used Observed O_3 data from 1990-2010 from 44 WOUDC sites



Xing et al, ACP, 2016

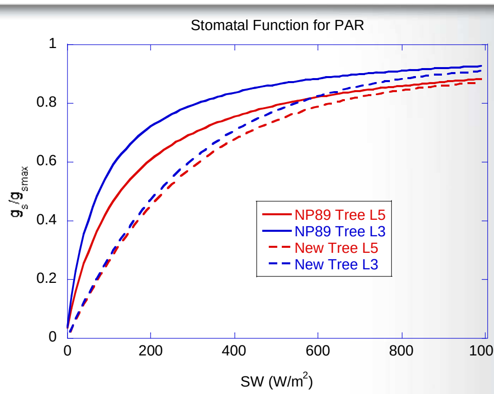
Comparison of Observed O_3 with Reference simulation and New PV scaling



Xing et al, ACP, 2016

Updates to WRF for AQ modeling

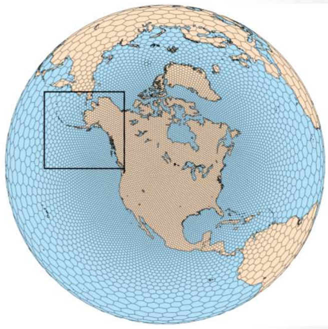
- WRFv3.7 (2015 release)
  - Updates to ACM2 PBL scheme
    - Different K_m and K_h ($Pr = K_m/K_h \neq 1$)
    - New eddy diffusivities for stable conditions
  - Updates to PX LSM :
    - Reduced heat capacity of vegetation (WRFv3.7)
      - Reduces predawn warm bias and post dawn cool bias

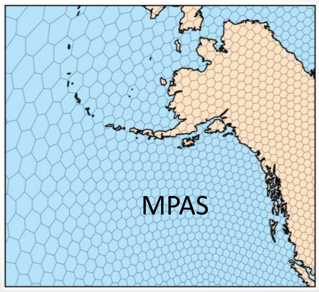


- WRFv3.8 (2016 release)
    - Further updates to stomatal conductance function for PAR (F1)
      - New F1 reduces LE late in the day which delays evening transition to stable surface flux
    - Revised Monin-Obukhov length calculation in pxsfclay to be more consistent w/ calculation in ACM2
- WRFv3.9 (2017 release)
  - MODIS LAI and VegFrac (fPAR) input (see Talk by Limei Ran this morning)
  - New soil resistance for evaporation in PXLSM

Vision for Next Generation Model

- **The Next Generation model will be a 1-D AQ component coupled to meteorology models**
  - Chemical tracers to be transported in meteorology model
  - Can couple to multiple Meteorology models
- **Three configurations of flexible systems:**
  - On-line global w/ seamless grid refinement (MPAS)
  - Online regional (WRF-AQ)
  - Offline regional (WRF-AQ with offline chem transport)
- **One dimensional AQ component**
  - Includes all vertical processes - vertical diffusion, advection, plume rise, gravitational settling, actinic flux
  - All 0-D processes - gas, aerosol, aqueous chemistry
  - Surface processes - biogenic emissions, dry dep/bidi, wind-blown dust
- **Transport in met models for online systems (adv, diffusion)**
  - Ensure mass conservation
  - Consistency with met parameters
  - Minimize numerical diffusion and dispersion

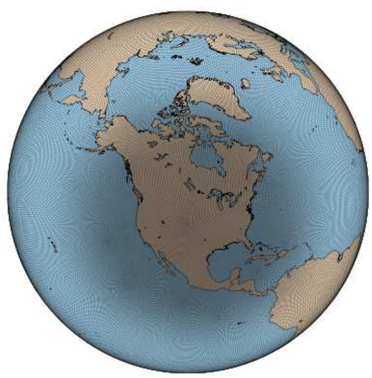




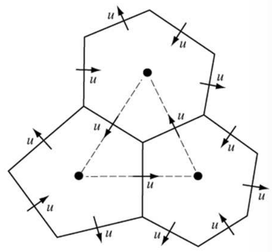
MPAS
Model for Prediction Across Scales

- Fully-compressible, non-hydrostatic dynamics
- Finite volume discretization on centroidal Voronoi (nominally hexagonal) grids
- Single global mesh with seamless refinement to local scales
- Latest version: MPAS 4.0 (released May 22, 2015)

MPAS uniform mesh (240 km)

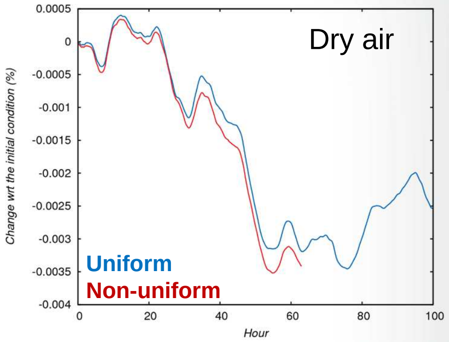


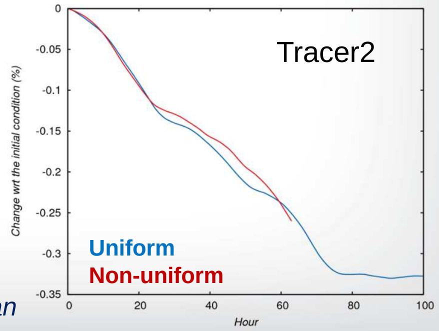
MPAS non-uniform mesh (92km – 25km)
Refinement over CONUS



MPAS development for NGAQM

- **Mass conservation experiments**
  - Ensure mass conservation on non-uniform grids
- **Physics implementations**
  - ACM2 PBL model
  - PX Land Surface Model
  - PX surface layer scheme
- **Data assimilation**
  - Four dimensional data assimilation
  - Soil moisture and temperature indirect assimilation



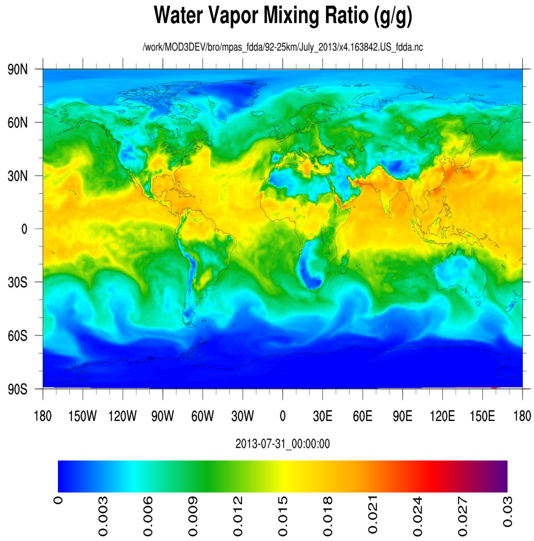


Courtesy of Hosein Foroutan

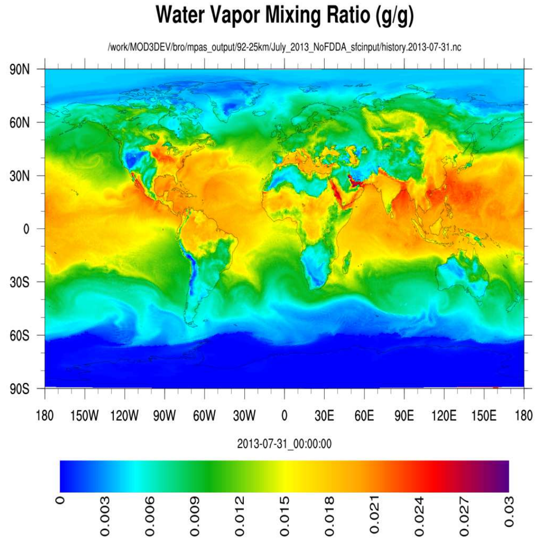
EPA United States Environmental Protection Agency

Without FDDA

FDDA Target (FNL) | *Simulation (+30 days)*



Layer 1



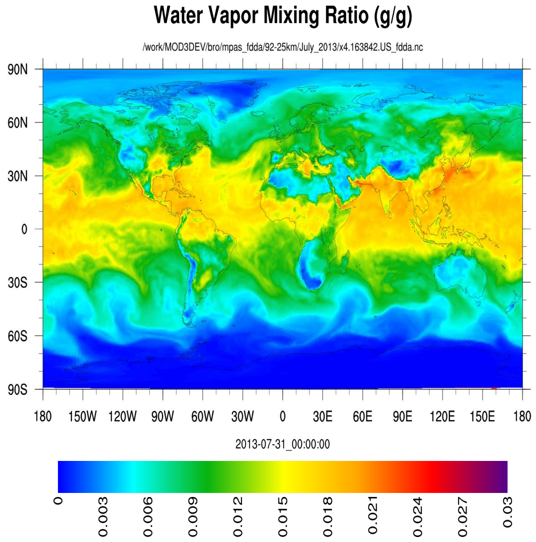
Layer 1

Office of Research and Development

Courtesy of Russ Bullock

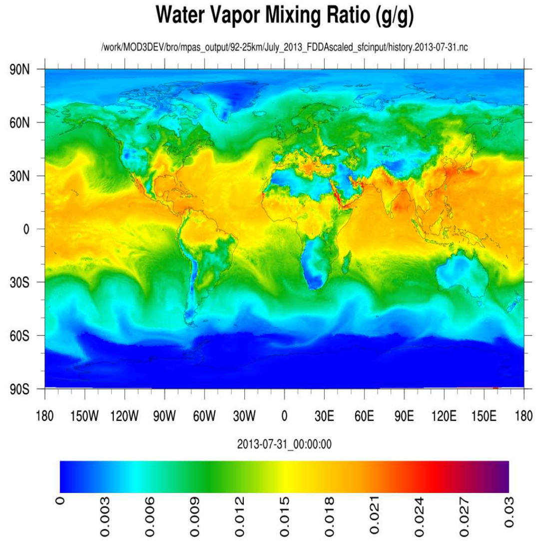
With FDDA

FDDA Target (FNL)



Layer 1

Simulation (+30 days)

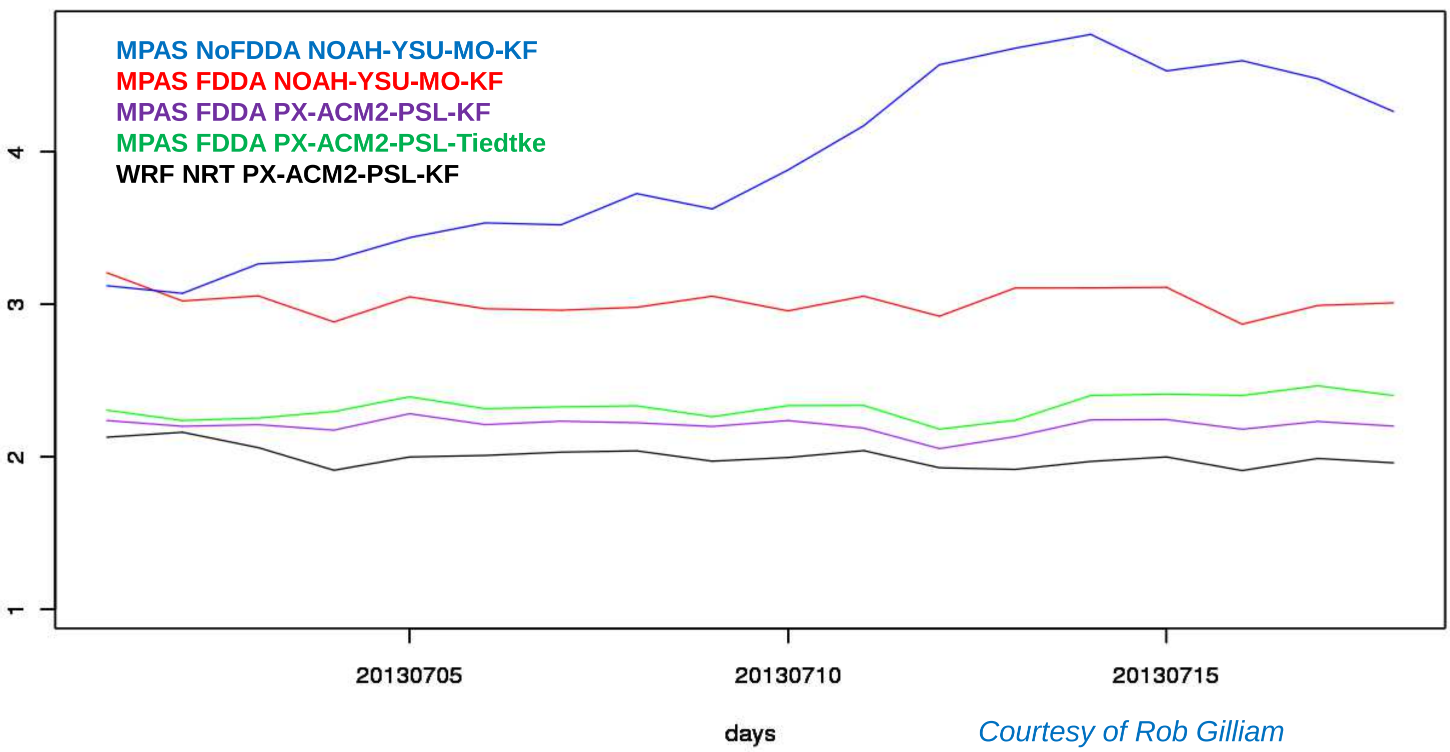


Layer 1

Office of Research and Development

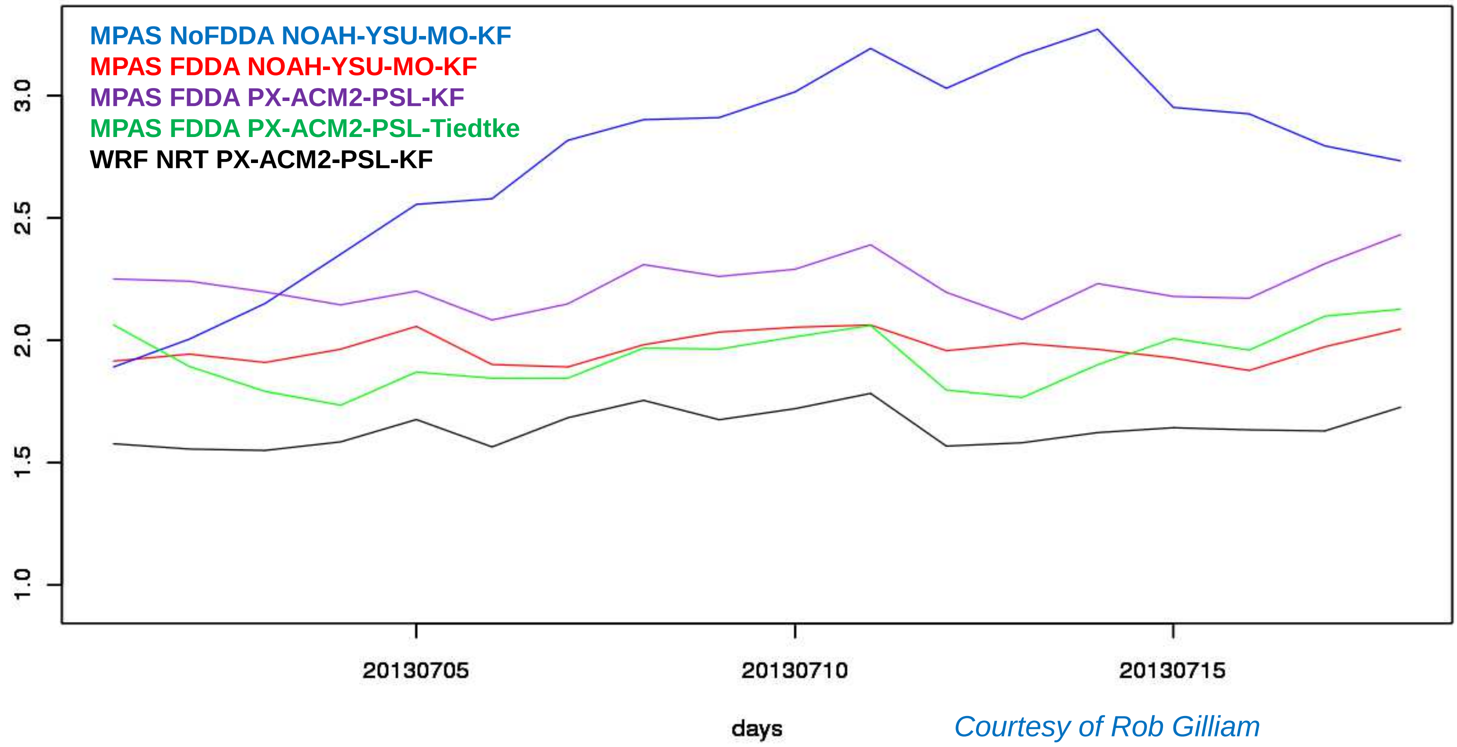
Courtesy of Russ Bullock

Daily 2-m Temperature RMSE (K) CONUS



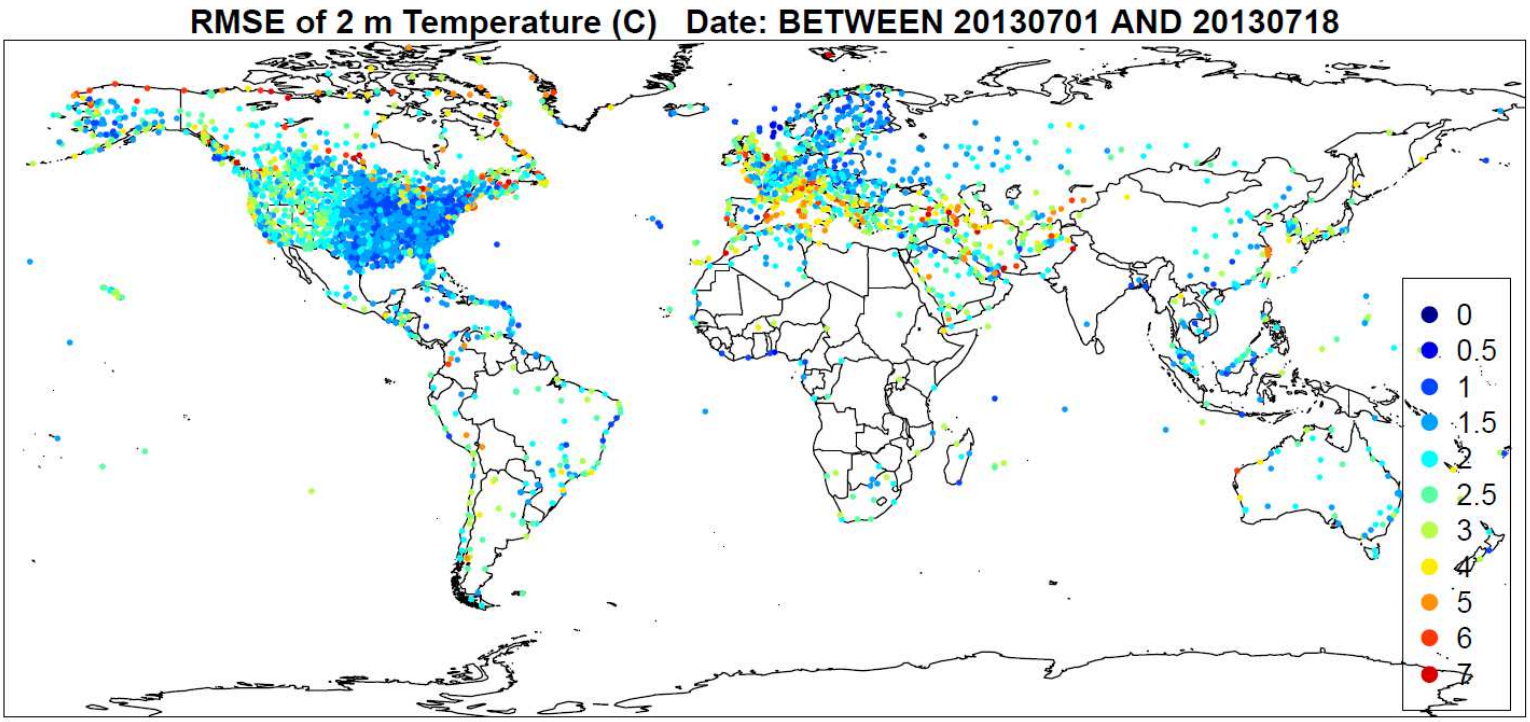
Courtesy of Rob Gilliam

Daily 2-m Mixing Ratio RMSE (g kg^{-1}) CONUS



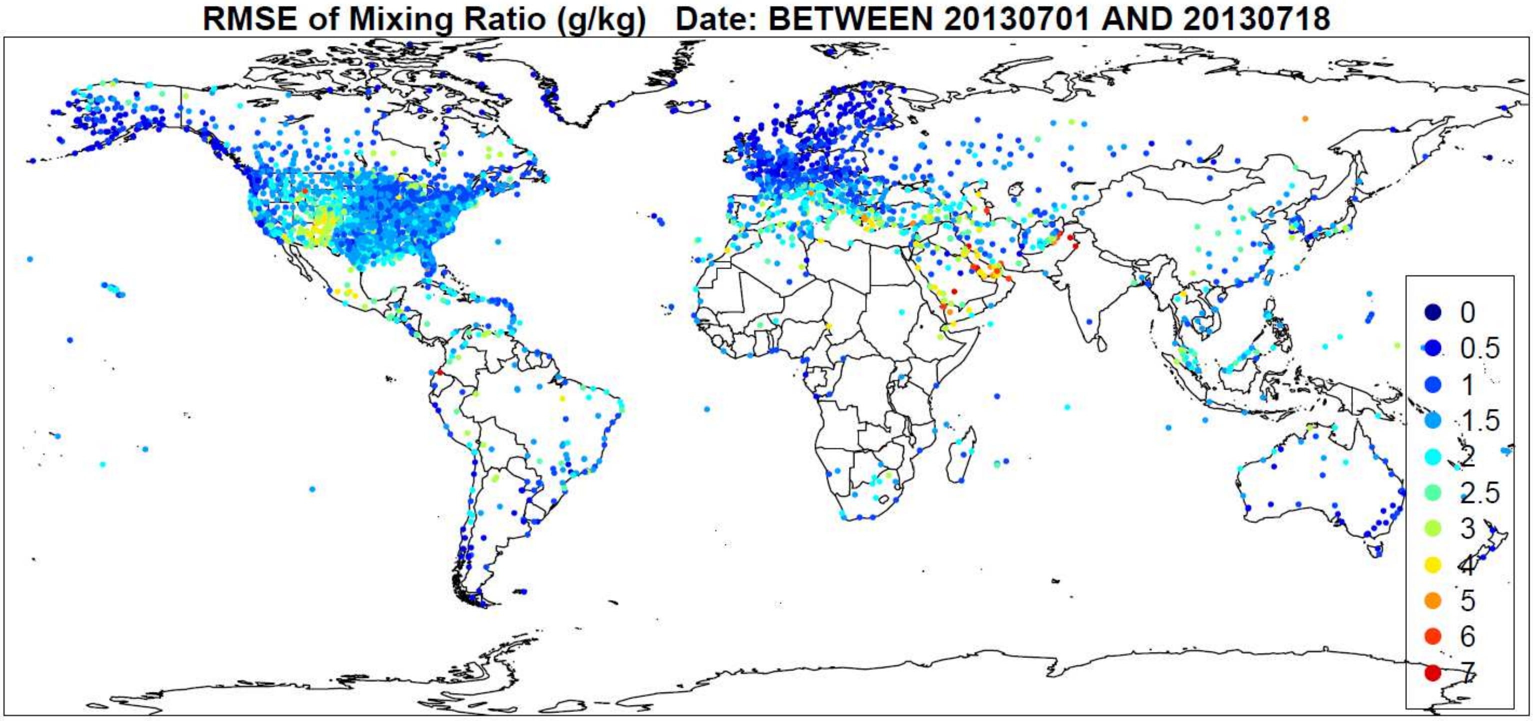
Courtesy of Rob Gilliam

MPAS FDDA PX-ACM2-PSL-Tiedtke



Courtesy of Rob Gilliam

MPAS FDDA PX-ACM2-PSL-Tiedtke



Courtesy of Rob Gilliam

Next Steps

- The Next Generation model will be a 1-D AQ component coupled to MPAS and WRF
  - Further physics improvements in MPAS
    - Update KF to include feedback to radiation
    - Update PX LSM to use MODIS vegetation products (LAI, fPAR) and fractional hi-res LULC
  - Developing new I/O system for AQ coupled to MPAS and WRF
  - Model design for 1-D AQ component and coupler
- Development of model science and algorithms will continue and expand to global scale
  - Condensed mechanisms linked to a detailed chemical mechanism (e.g. MCM)
  - Continue advances in organic aerosols and new particle formation
  - Develop integrated cloud model w/ convective transport, microphysics, aqueous chem, aerosol-cloud interactions
  - Emission process modeling for global coverage – (dust, biogenic, bidirectional flux, fires)
- Continued support and updates to CMAQ until NGAQM is ready

附錄七　**Source apportionment of fine particulate matter in Yunlin County in Taiwan**

Source Apportionment of Fine Particulate Matter in Yunlin County, Taiwan

Yi-Ju Lee and Fang-Yi Cheng
Department of Atmospheric Science, National Central University

Oct 25, 2015

Outline

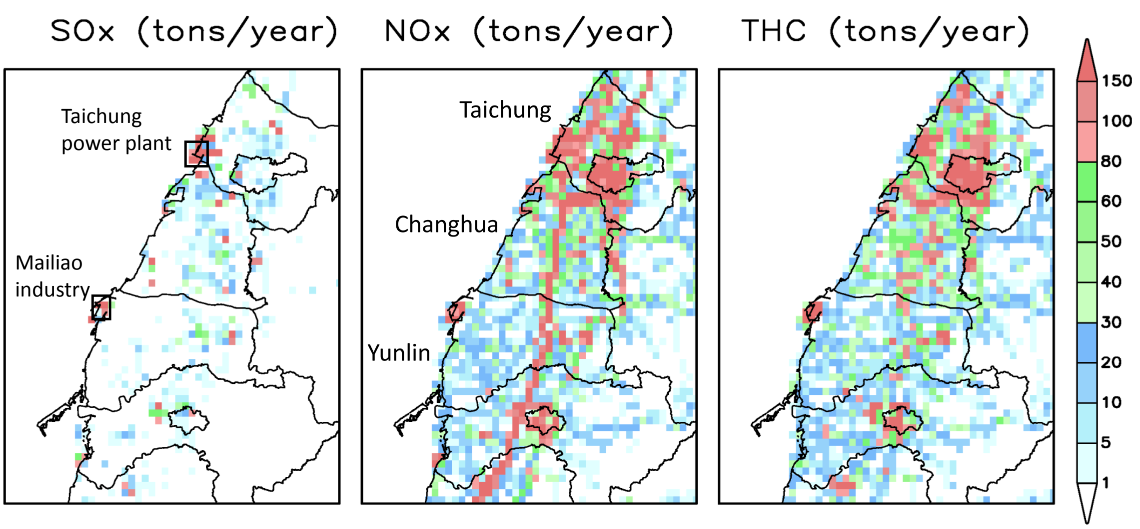
- Introduction and Motivation
- Model configuration
- Experiments
- Discussion
- Conclusion
- Reference

Introduction and Motivation

Introduction

- Yunlin County is located in central portion of western Taiwan.
- Major emissions : industry, vehicle exhausts and burnings of agricultural wastes

Taiwan Emission Inventory



Objective

- Hsu and Cheng (2016) showed that $PM_{2.5}$ concentrations in Yunlin County can be affected by different weather patterns.

- The local circulation might transport the air pollutants toward the inland areas and induce high concentration.

Objective: to investigate main emission source that contributes to $PM_{2.5}$ concentration in Yunlin County under different weather conditions using CMAQ source apportionment technique.

Source apportionment

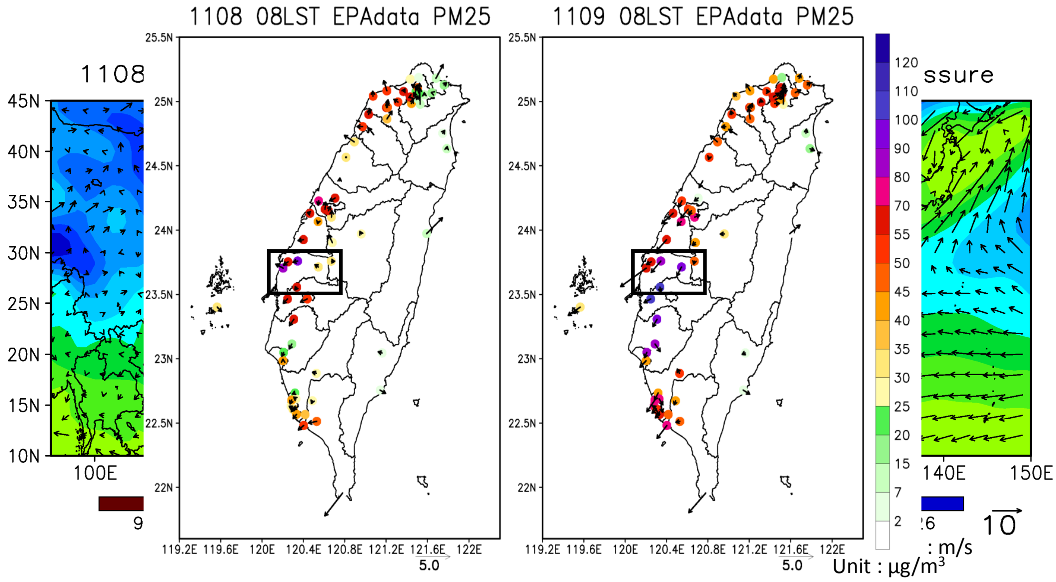
SA provides information as to the most important potential sources of $PM_{2.5}$.

- Brute Force Method (BFM) – source sensitivity
  Comparing results of base model and model with perturbed emissions.

- Integrated Source Apportionment Method (ISAM) – tag species
  Tracking tagged species from emission source groups and/or regions.
  Computational time is less then BFM.

Description of simulation episode (11/8 – 11/9, 2015)

- Nov 8 was associated with weak synoptic weather condition.
- Nov 9 was affected by weak northeasterly monsoonal flaw.
- $PM_{2.5}$ concentration is higher on Nov 9 than on Nov 8.



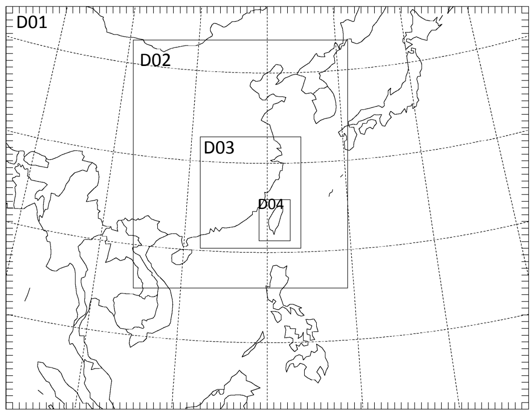
Model configuration

Model configuration

WRFv3.7.1	D01	D02	D03	D04
Resolution	81km	27km	9km	3km
Reanalysis data	NCEP FNL (1°x1°, 6 hour)			
Vertical levels	48 (top 5000Pa)			
Boundary-layer scheme	YSU			
Observational nudging	X			V

CMAQv5.0.2		
Resolution		3km
Vertical levels		20
Meteorology		WRFv3.7.1 / MCIPv4.2
Emission	Anthropogenic	Taiwan emission inventory
	Biogenic	MEGANv2.04
Chemical mechanism		CB05tucl
Aerosol chemistry		AERO6

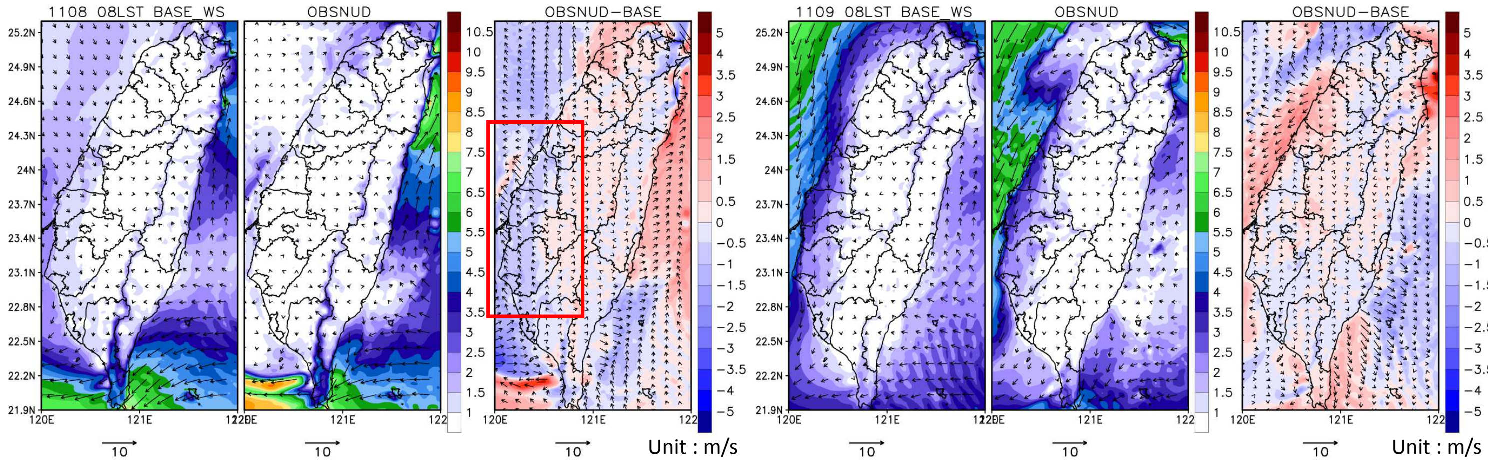
- Simulation periods :
  2015/11/03 00UTC – 11 00UTC
- OBSnudging : every hour
  CWB and EPA monitoring stations data
  Temperature and wind



Comparison of simulated wind fields

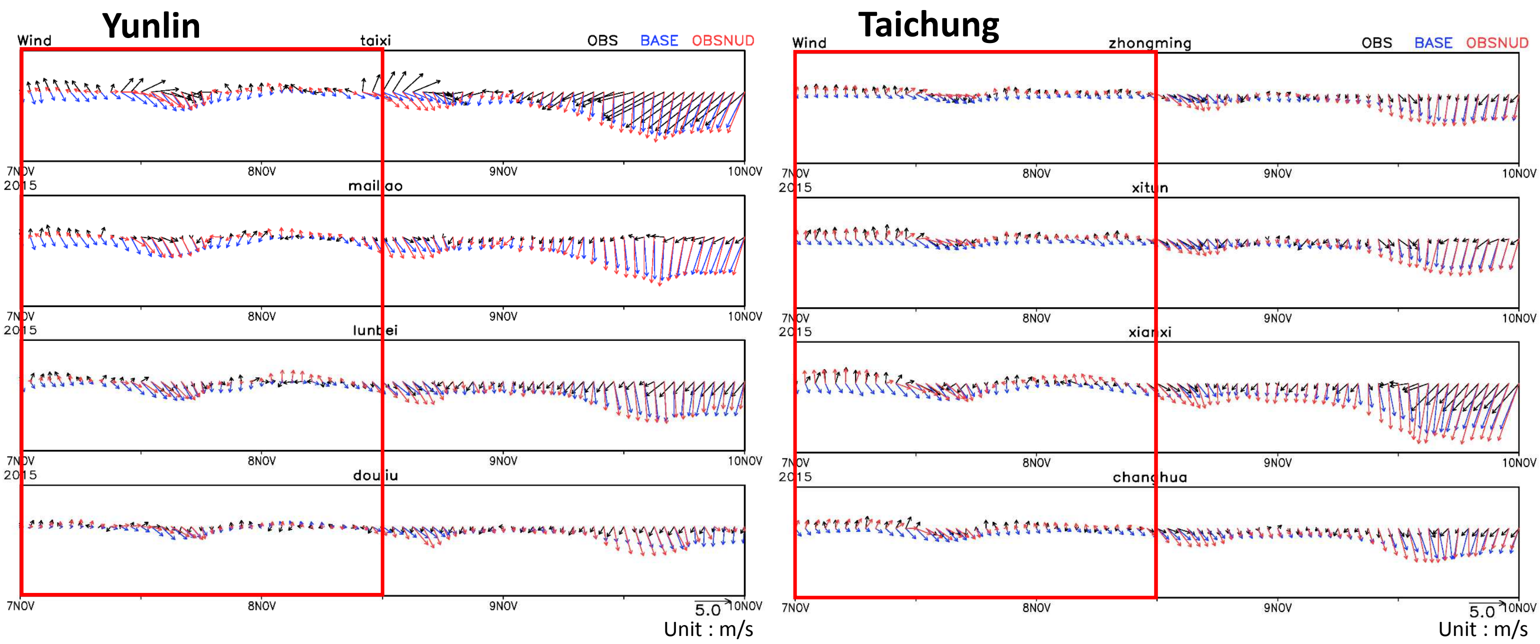
- Wind speed was weaker on Nov 8 due to weak synoptic weather forcing.
- There was a weak northeasterly monsoonal flow on Nov 9.
- OBSNUD simulates lower wind speed than base case in central portion of western Taiwan.

1108 08LST **1109 08LST**



Evaluation of simulated wind fields

- WRF simulation with OBSnuding technique improves the simulation of wind fields showing weaker wind speed and better land-sea breeze flow.

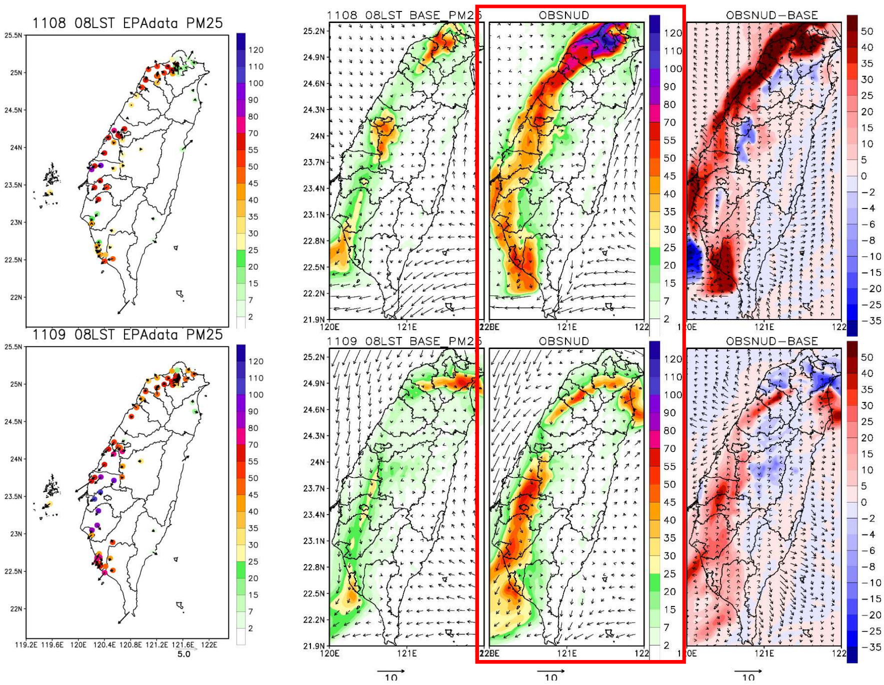


Comparison of simulated $PM_{2.5}$ concentration

- CMAQ simulation with OBSNUD shows weaker wind fields that accumulates more $PM_{2.5}$ near emission source region.

1108 08LST

1109 08LST



Color unit : μg/m³
Bar unit : m/s

Design of Source Apportionment Experiments

Simulation periods: 2015/11/03 00UTC – 11 00UTC

- Taichung power plant

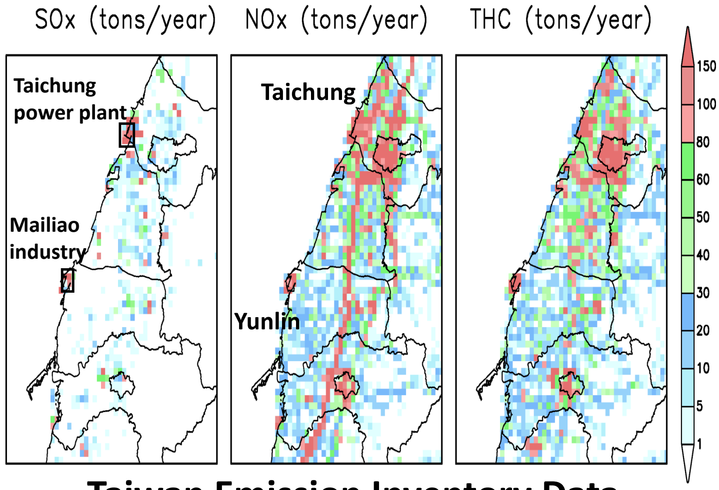
The largest coal-fired power plant in the world

- Yunlin and Taichung

Local emissions and metropolitan area

- Mailiao industrial complex

The largest emission source in Yunlin



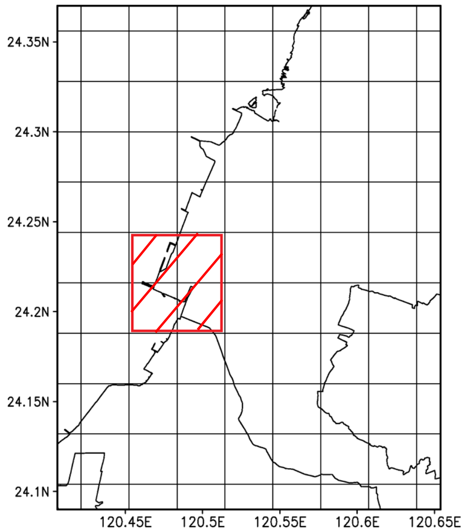
Taiwan Emission Inventory Data

Discussion

1St Source Apportionment Experiment

- Taichung power plant : point source
  - BFM : zero-out
    TCplant.SOX
    TCplant.NOX
  - ISAM
    Sulfate and nitrate

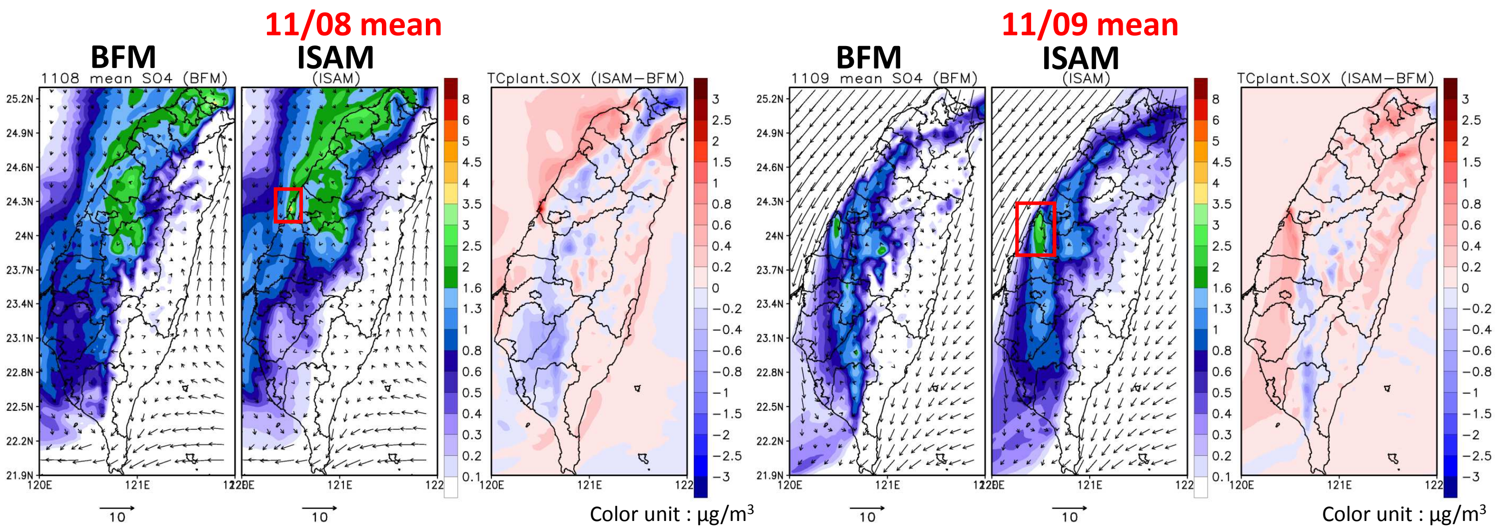
	tons/year	region.%
$PM_{2.5}$	1293.54	72.6%
SO_X	15319.21	93.2%
NO_X	24923.36	95.0%
CO	3969.47	93.6%



→ compare results between BFM and ISAM

BFM vs ISAM (TCplant: SO_X-SO_4)

- Simulated patterns were similar between BFM and ISAM.
- Emission source contribution area were different on Nov 8 and Nov 9.
- ISAM calculated higher contributions (about 0.4-0.6 μg/m^3) in Yunlin and location of maximum value was closer to emission sources than BFM.



Color unit : μg/m^3
Bar unit : m/s

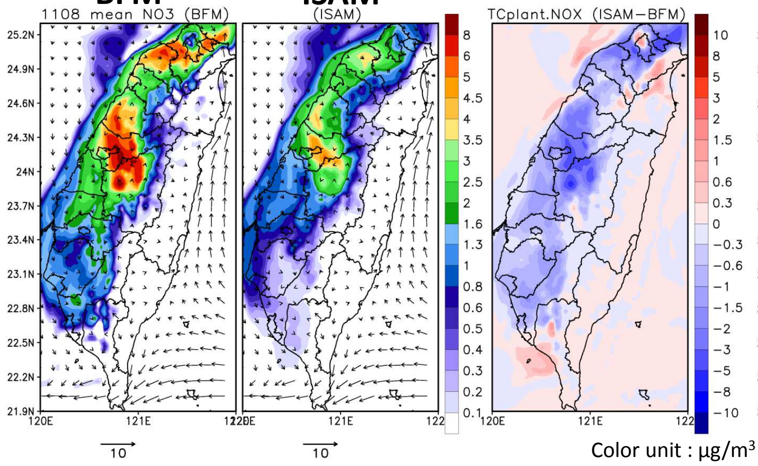
Color unit : μg/m^3
Bar unit : m/s

BFM vs ISAM (TCplant: NO_X-NO_3)

- ISAM calculated lower contributions (about 1.5-2 μg/m^3) in Yunlin than BFM.
- The discrepancy was due to higher nonlinearity in NO_X chemistry.
- ISAM calculates the source contributions, but BFM estimates the responses of zero-out concentration.

11/08 mean

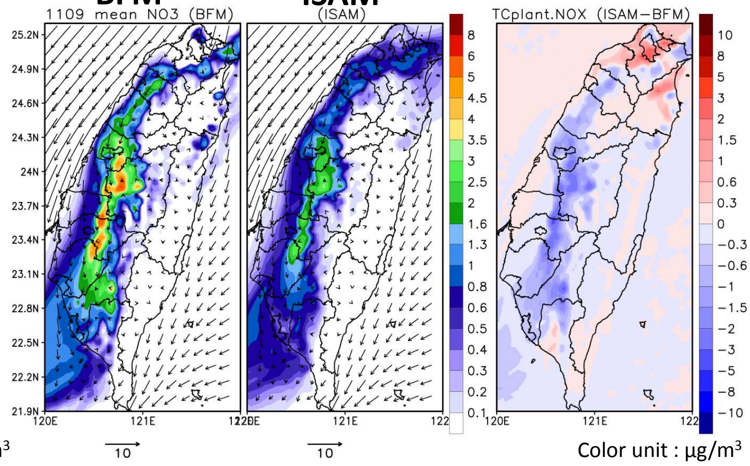
BFM **ISAM**



Color unit : μg/m^3
Bar unit : m/s

11/09 mean

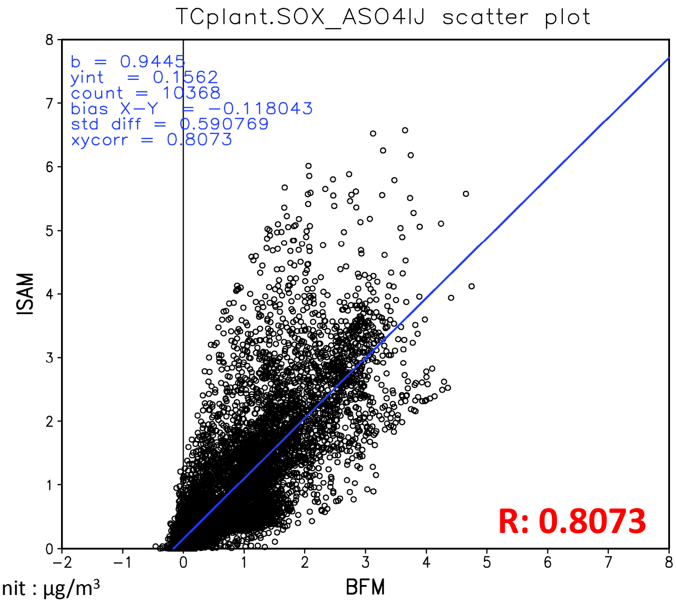
BFM **ISAM**



Color unit : μg/m^3
Bar unit : m/s

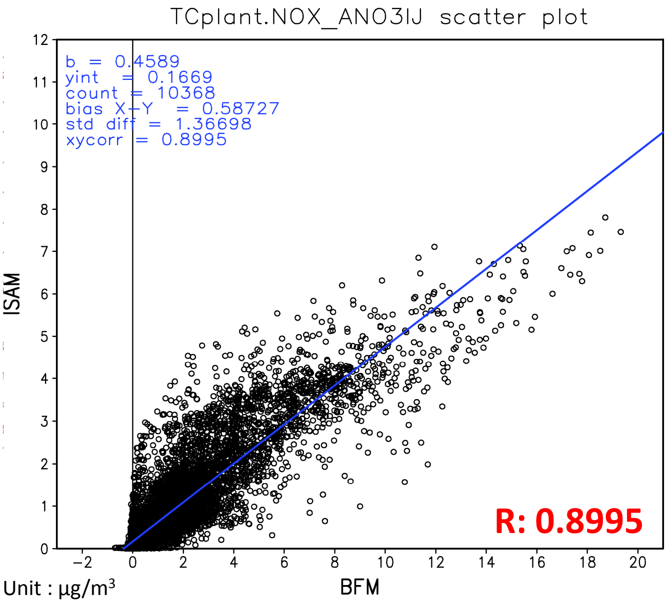
BFM vs ISAM

TCplant: SO_X – ASO_4IJ



Unit : μg/m^3

TCplant: NO_X – ANO_3IJ



Unit : μg/m^3

2nd Source Apportionment Experiment

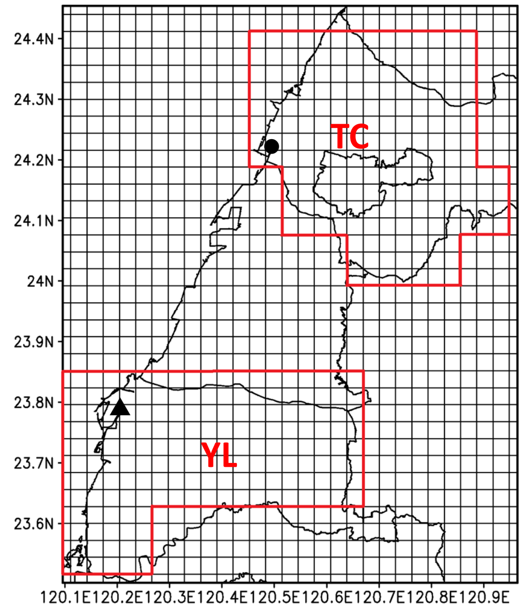
- Yunlin and Taichung
  - ISAM only

    Point, area and line sources

    Sulfate and nitrate

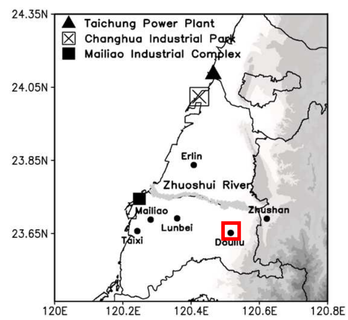
    Yunlin (YL) and Taichung (TC)

In Taichung,
only consider the emission from metropolitan area

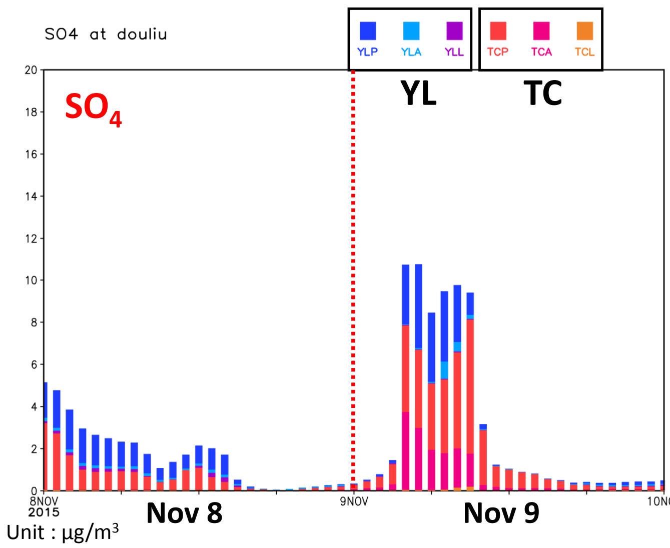


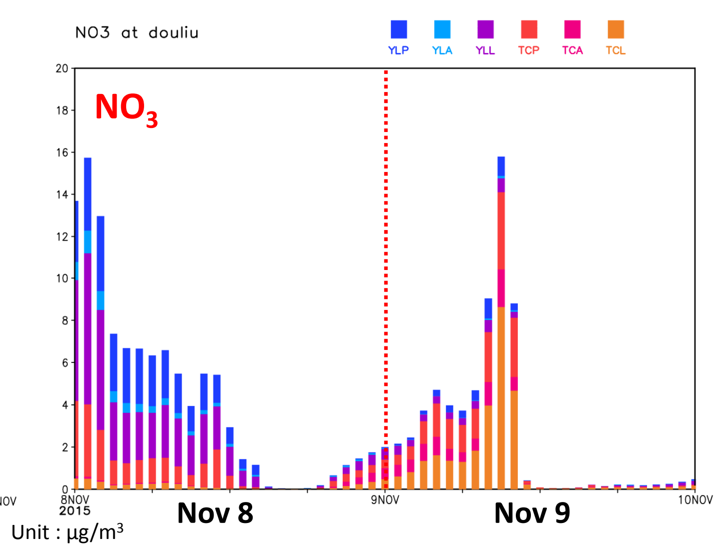
▲ Mailiao industrial complex ● Taichung power plant

Source apportionment at Douliu, Yunlin County



- On 11/08 (with weak synoptic), emissions are mainly from Yunlin
- On 11/09 (with NE flow), emission are mainly from upwind of Taichung.
- In addition to point sources, sulfate is also contributed from area and nitrate from line emission sources.





3rd Source Apportionment Experiments

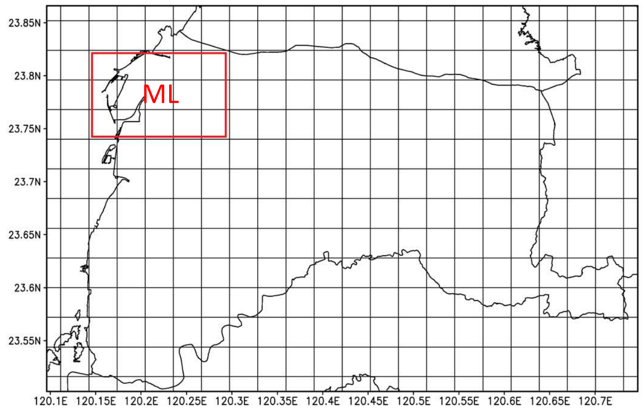
- Mailiao industrial areas
  - ISAM only

    Point source

    Sulfate and nitrate

    Mailiao (ML)

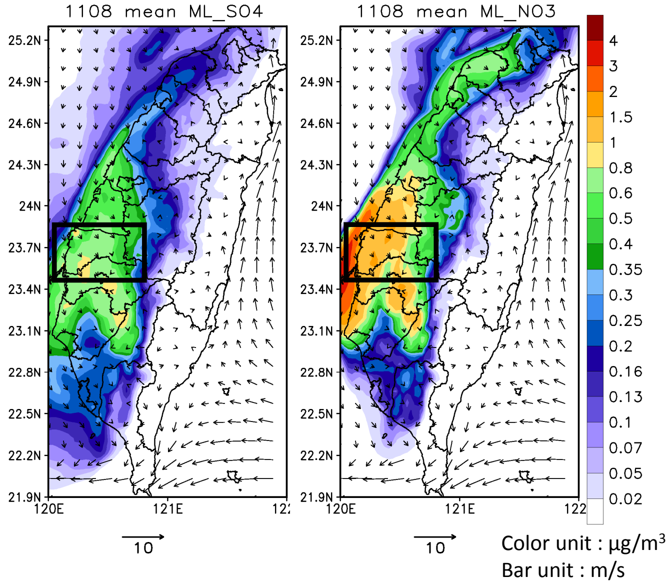
	tons/year
$PM_{2.5}$	717.84
SO_X	5726.90
NO_X	14924.29



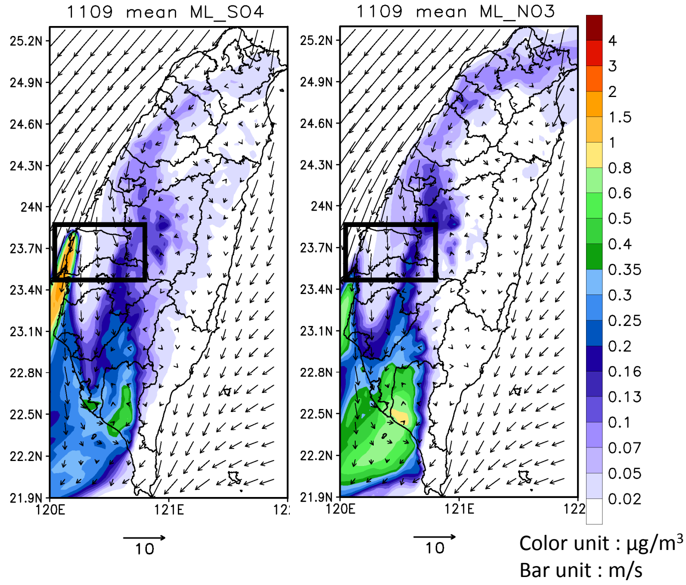
3rd SA experiment: Source contributions from Mailiao Emissions

- On 11/08 (with weak synoptic weather), Mailiao emissions mainly affect Yunlin and surrounding county areas, and even toward inland area due to onshore sea breeze.
- On 11/09 (with NE flow), Mailiao emissions mainly affect downwind southern Taiwan.

1108 mean



1109 mean



Conclusion

Conclusion

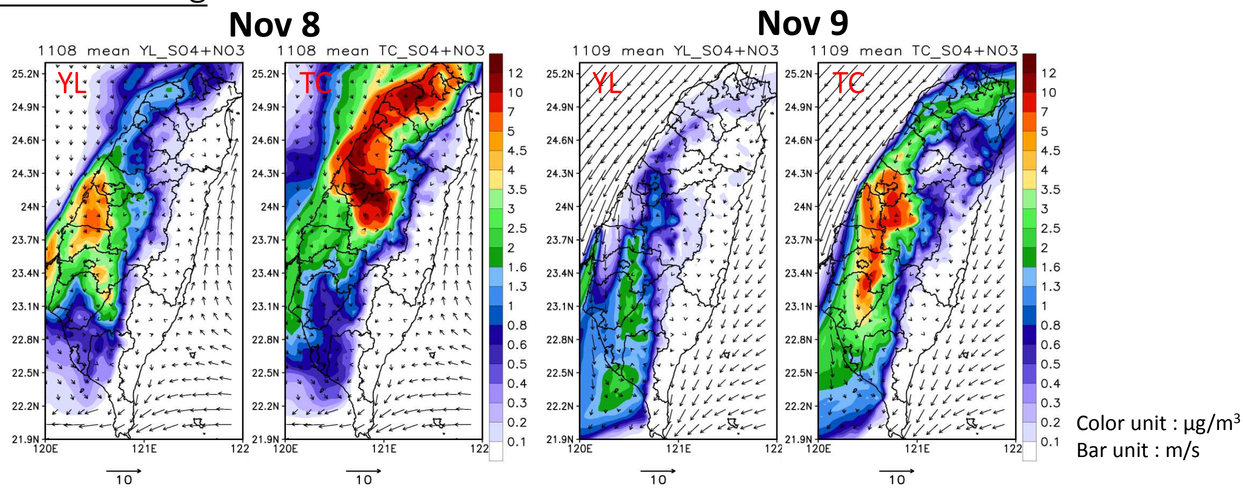
- CMAQ with **BFM** and **ISAM** are applied to investigate emission sources contributions to $PM_{2.5}$ concentrations in Yunlin from Nov 8 to Nov 9, 2015.

- Results from BFM and ISAM are close to each other.
  - Contribution of **SO_X to sulfate** calculated by ISAM was higher than by BFM, but the contribution of **NO_X to nitrate** was opposite.
  - Discrepancy between BFM and ISAM was larger in nitrate because of higher nonlinearity in the NO_X chemistry.

- In terms of sulfate, the maximum calculated by **ISAM** is higher and closer to emission sources than BFM.

Conclusion

- Nov 8 was with weak synoptic weather and $PM_{2.5}$ in Yunlin County are mainly contributed from local Yunlin emission sources.
- Nov 9 was affected by by northeasterly monsoonal flow and $PM_{2.5}$ are mainly contributed from upwind Taichung area.



- $PM_{2.5}$ concentration in Yunlin County can be contributed from different emission source region under different weather conditions.

Reference

- Hsu, Chia-Hua, Fang-Yi Cheng. (2016). Classification of weather patterns to study the influence of meteorological characteristics on $PM_{2.5}$ concentrations in Yunlin County, Taiwan. Submitted.
- Kwok, R. H. F., Napelenok, S. L., & Baker, K. R. (2013). Implementation and evaluation of PM 2.5 source contribution analysis in a photochemical model. *Atmospheric Environment*, *80*, 398-407.

附錄八　**NAQFC CTM upgrade to CMAQv5.0.2**

National Air Quality Forecasting Capability CTM upgrade to CMAQ5.0.2

EMC – team
- Jeff McQueen
- Jun Wang
- Jianping Huang
- Perry Shafran
- Ho-chun Huang

ARL – team
- Pius Lee
- Youhua Tang
- Li Pan
- Hyuncheol Kim
- Daniel Tong

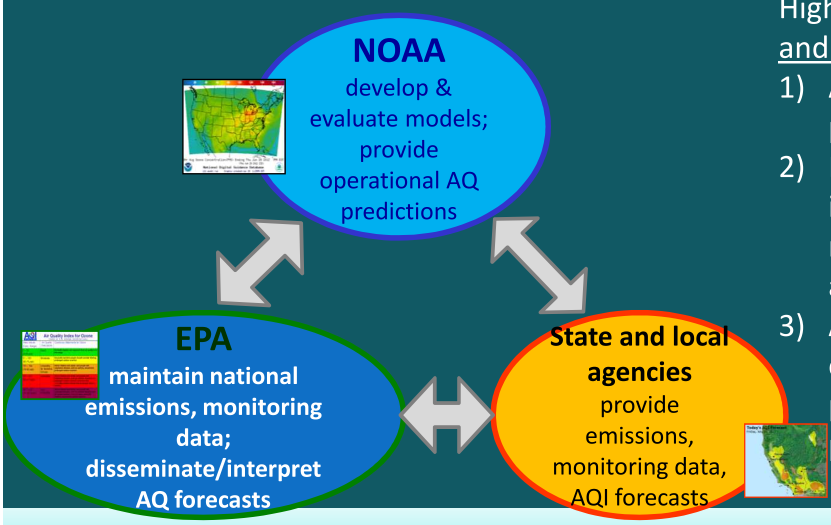
ESRL – team
- James Wilczak
- Dave Allured
- Irina Djalalova

Program management
- Ivanka Stajner (Manager)
- Sikchya Upadhayay

Collaborators:
- Sarah Lu (SUNY)
- Luca Delle Monache, Gabriele Pfister (NCAR)

Impact and Partnerships

- Implementing NOAA/NWS National Air Quality (AQ) Forecast Capability operationally to provide graphical and numerical guidance, as hourly gridded pollutant concentrations, to help prevent loss of life and adverse health impacts from exposure to poor AQ.
  - Exposure to fine particulate matter and ozone pollution leads to premature deaths, of over 50,000 annually in the US (Science, 2005; recently updated to 100,000 deaths; Fann, 2011, *Risk Analysis*).
- Direct impact on reducing loss of life: AQ forecasts have been shown to reduce hospital admissions due to poor air quality (Neidell, 2009, J. of Human Resources)
- NOAA's AQ forecasting leverages partnerships with EPA, under authorization of 15 USC 313, and complies with Congressional direction to NWS for building and implementing operational AQ forecasting.

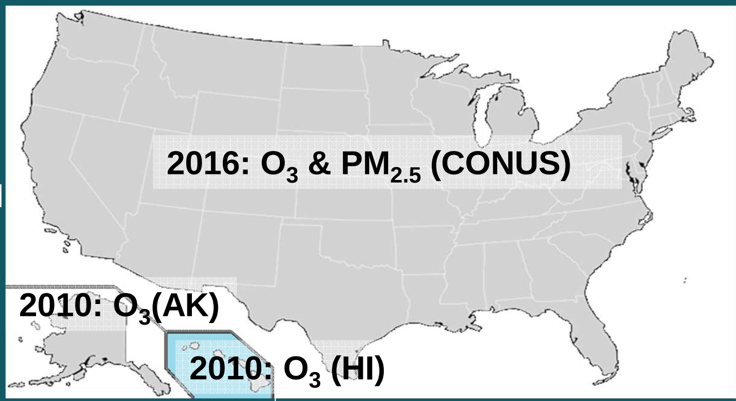


Highlights of recent feedback from state and local AQ forecasters:
1) AQ forecasters rely on NAQFC products to issue AQ forecasts,
2) NAQFC ozone predictions have improved substantially this year relative to previous years over large areas of Eastern US,
3) AQ forecasters urged NOAA to continue producing ozone predictions and prototype particulate matter predictions.

Operational NAQFC

Chemical Transport Model:
▪**CMAQ4.6** for **CONUS, AK & HI**
- CB05 gas chemistry
- Aero4 aerosol chemistry
- LBC: monthly varying GEOS-CHEM
  Dynamic LBC for dust derived from NGAC

- **O_3 product dissemination: TOC**



Max Daily 8h (MDA8) O_3 threshold 70ppb
24 h averaged $PM_{2.5}$ threshold 35 μg/m^3
Basic metric: Bias, RMSE, and % Hit Rate

Lee, McQueen, Stajner et al., *Weather & Forecasting* 2016
DOI: WAF-D-15-0163.1

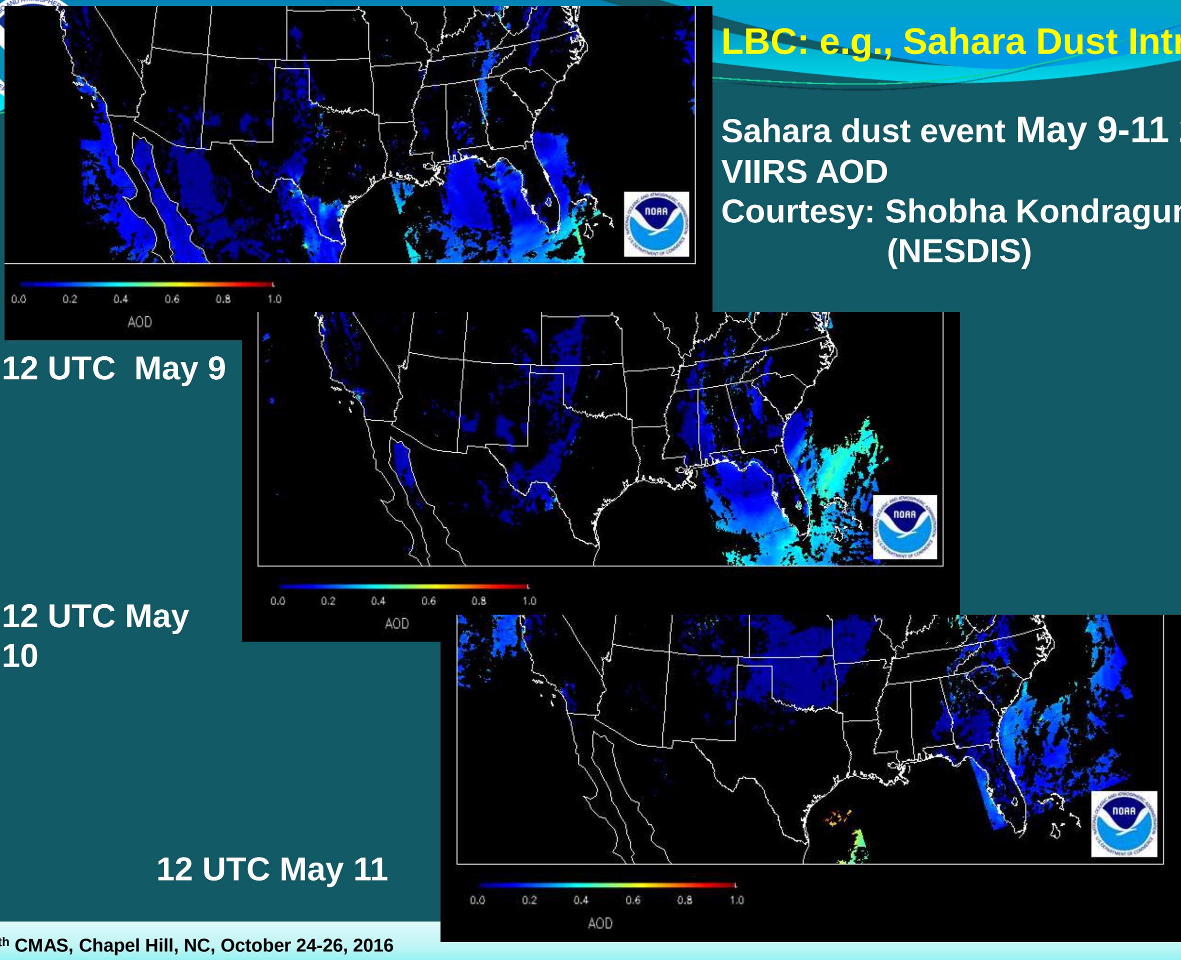
Strong interest for NOAA $PM_{2.5}$ forecast. E.g., Fann et al., Risk Analysis 2011: "Studies by American Cancer Society and National Mortality & Morbidity Air Pollution Study showed that 130,000 and 4,700 died of $PM_{2.5}$ and O_3; respectively in 2005".

Emission Data Sources for CMAQ 5.0.2

- **Area Sources**
  - **US EPA 2011 NEIs;**
  - **Canada 2006 Emission Inventories (in NEI2011 package);**
  - **Mexico 2012 EI for six border states (in NEI2011 package);**
  - **New US residential wood combustion and oil and gas sectors;**
  - **Snow/Ice effect on fugitive dust emissions;**
- **Mobile Sources (onroad)**
  - **NEI 2005 projected to 2011 using Cross-State Air Pollution Rule (CSAPR) projection for US sources and then adjusted further to the forecast year using trends from surface and satellite observations from 2011 to 2014;**
  - **Canada 2006 Emission Inventories;**
  - **Mexico 2012 EIs;**
- **Point Sources (EGUs and non-EGUs)**
  - **Baseline emissions from NEI2011;**
  - **US EGU sources updated with 2014 Continuous Emission Monitoring (CEM);**
  - **Projected into forecast year using DOE Annual Energy Outlook projection factors;**
- **Natural Sources**
  - ***Terrestrial biogenic emission:* BEIS model v3.14;**
  - ***Sea-salt emission:* CMAQ online Sea-salt emission model based on 10m wind;**
  - **Fire emissions based on HMS fire detection and BlueSky emission model;**
  - **Windblown dust emission: FENGSHA model;**

LBC: e.g., Sahara Dust Intrusion

Sahara dust event May 9-11 2015
VIIRS AOD
Courtesy: Shobha Kondragunta (NESDIS)



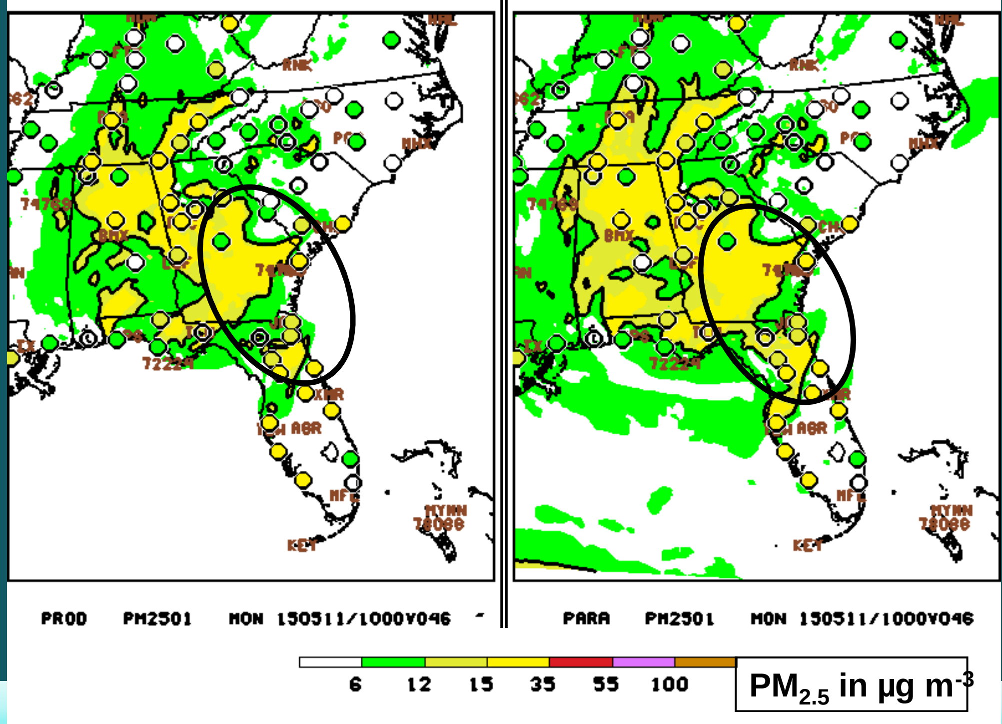
12 UTC May 9

12 UTC May 10

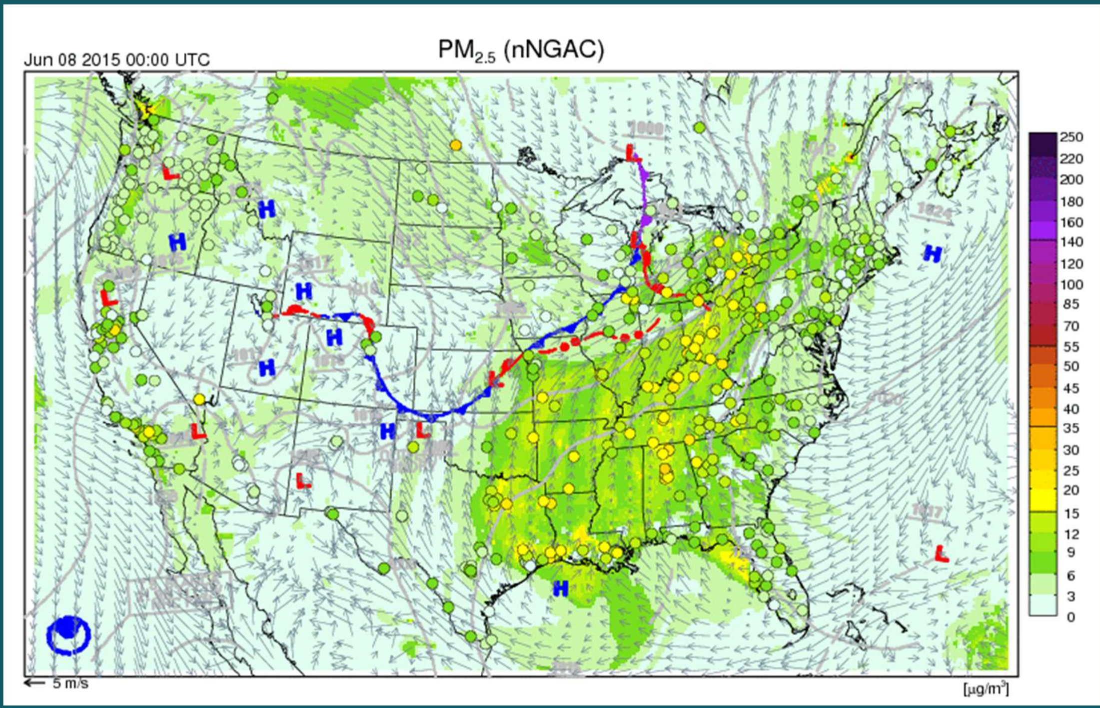
12 UTC May 11

Surface concentration of $PM_{2.5}$ at 10 UTC May 11 2015: modeled (background shading), measured (filled circle)

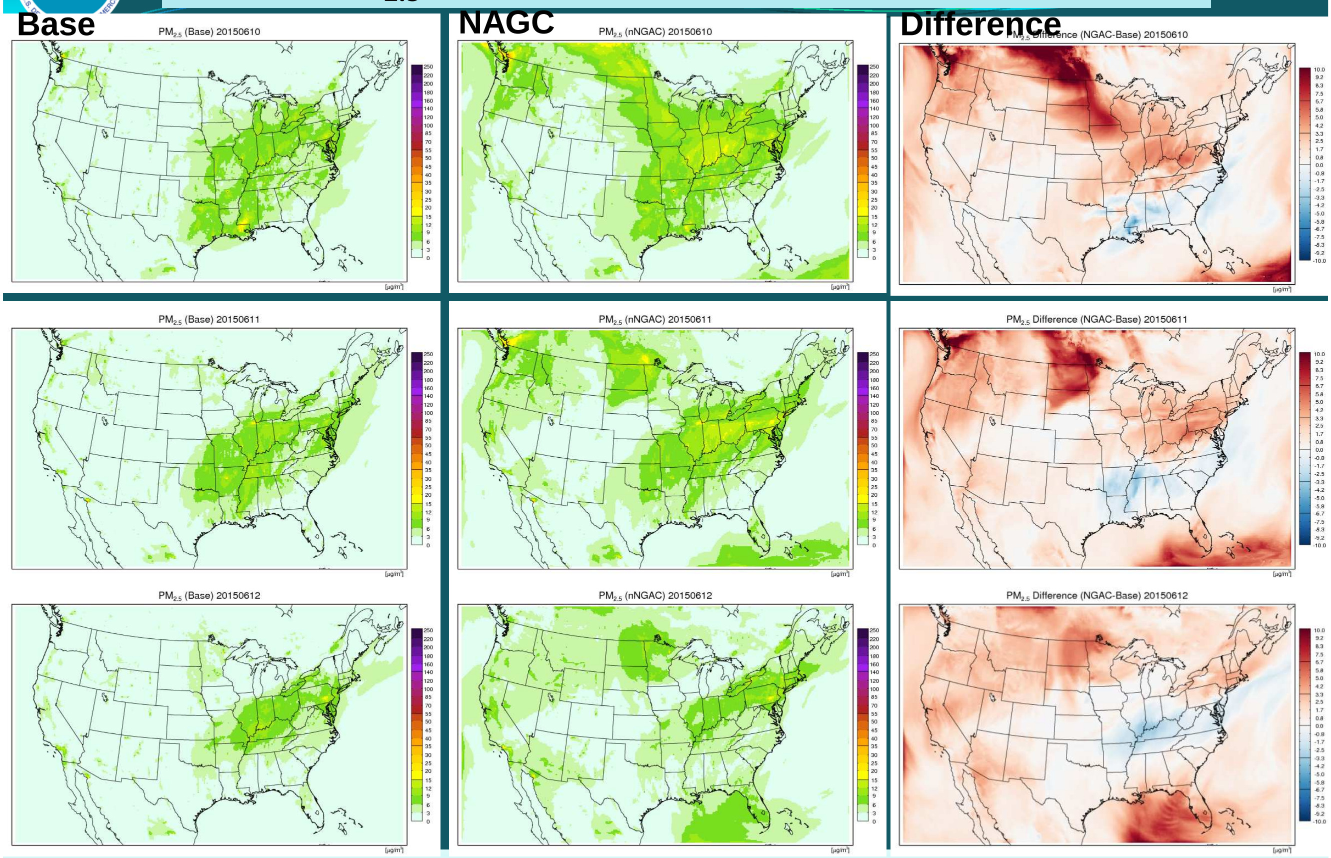
Without dynamic boundary condition | **With dynamic boundary condition**



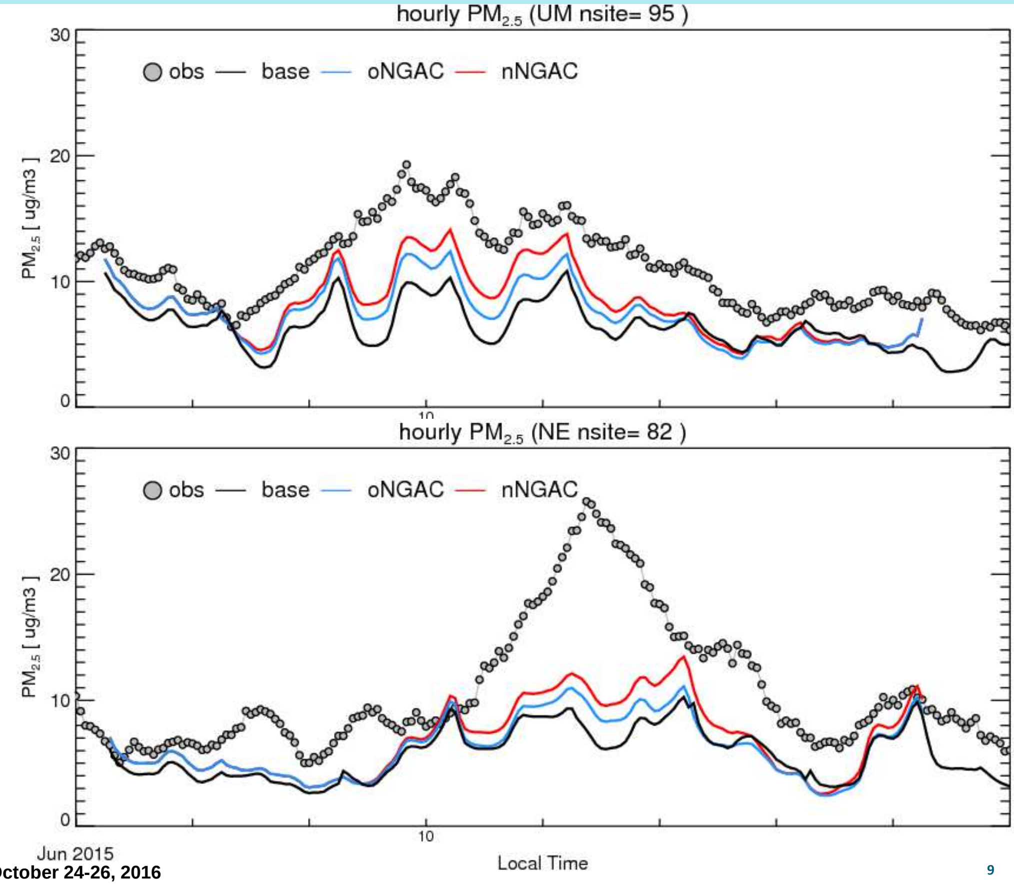
Analysis of the June 9-12 2015 Canadian fire: Surface $PM_{2.5}$ with frontal passages



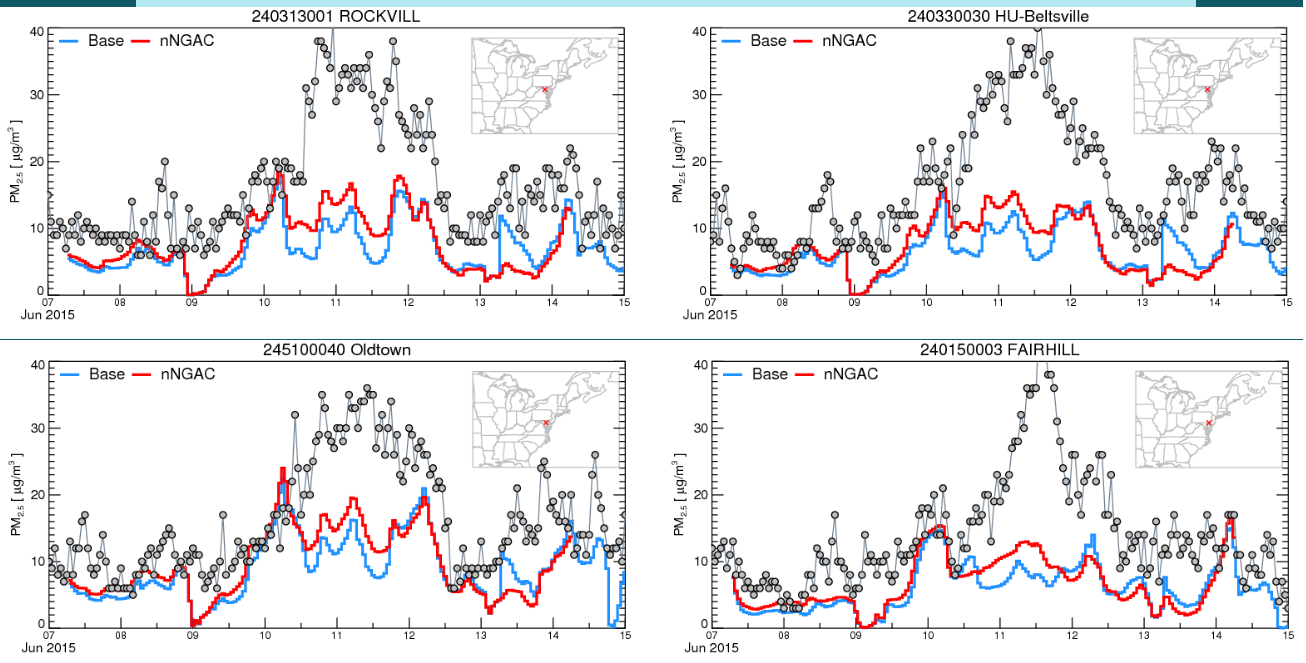
Analysis of the June 9-12 2015 Canadian fire (cont'd) Surface $PM_{2.5}$ with frontal passages



Analysis of the June 9-12 2015 Canadian fire (cont'd) Surface $PM_{2.5}$ with frontal passages

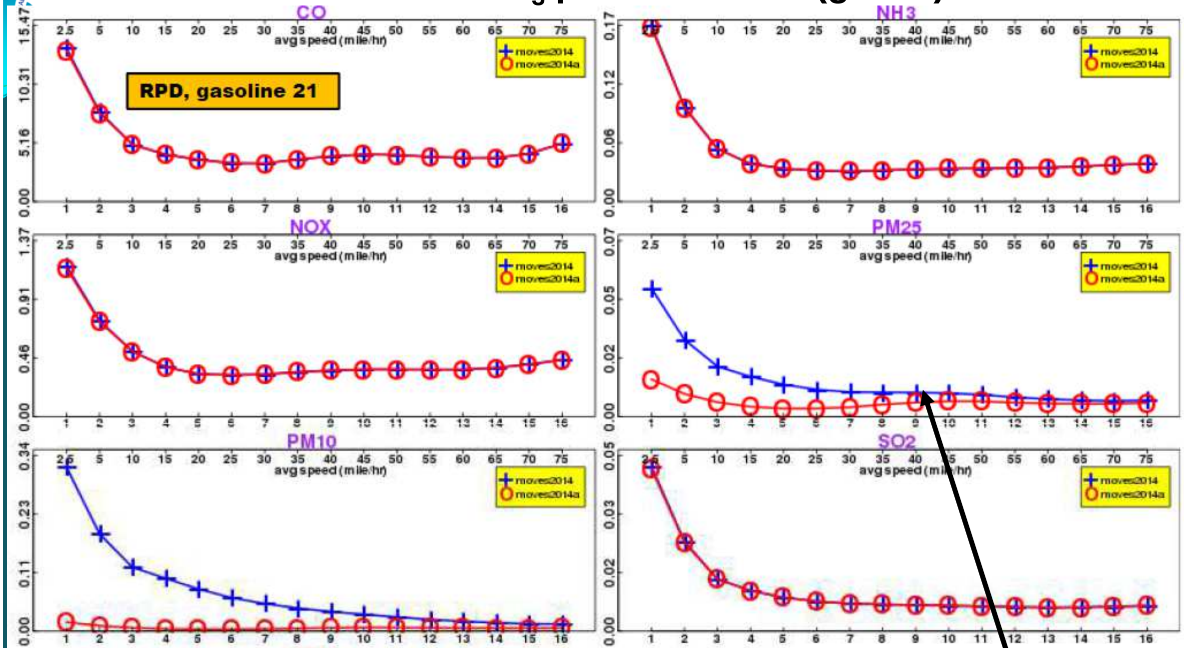


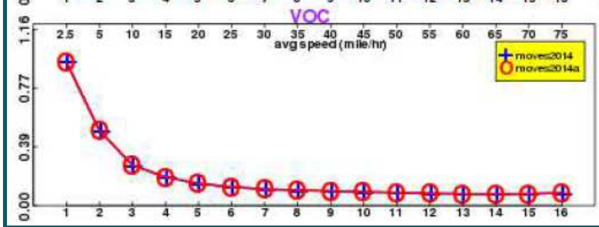
Analysis of the June 9-12 2015 Canadian fire (cont'd) Surface $PM_{2.5}$ with frontal passages



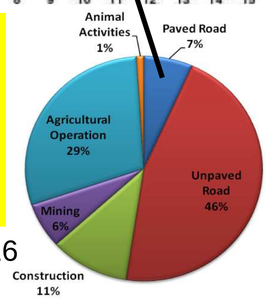
Showed improved skills and awaits NGAC upgrades

MOVES2014a has similar O_3 precursor rate (g/mile) as MOVES2014





Helps $PM_{2.5}$ but exacerbate O_3 over-prediction

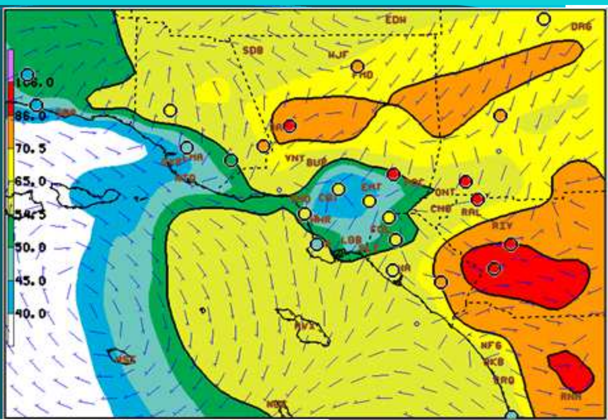


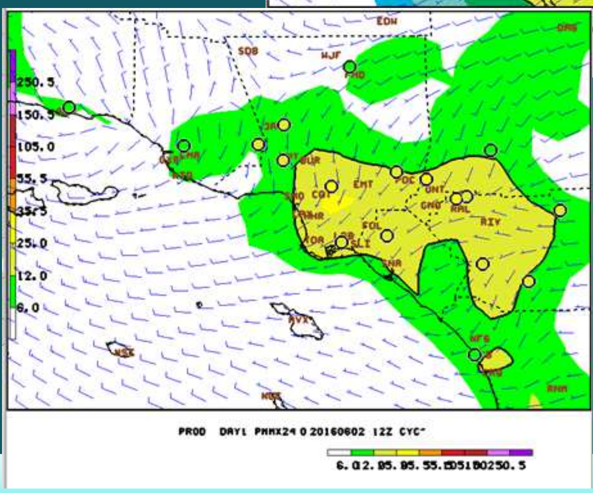
Pie chart shows % of $PM_{2.5}$ emission

Courtesy: Jin-Sheng Lin et al., VDEQ, 2016

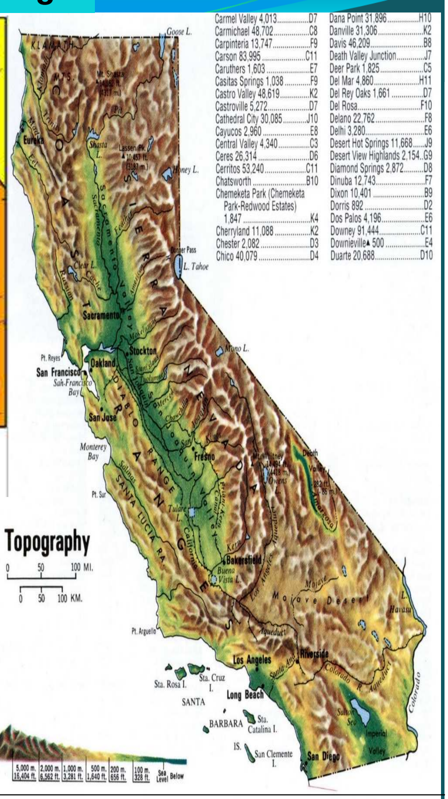
complex terrain e.g., South Coast poses challenge

MDA8 O_3 on June2 2016





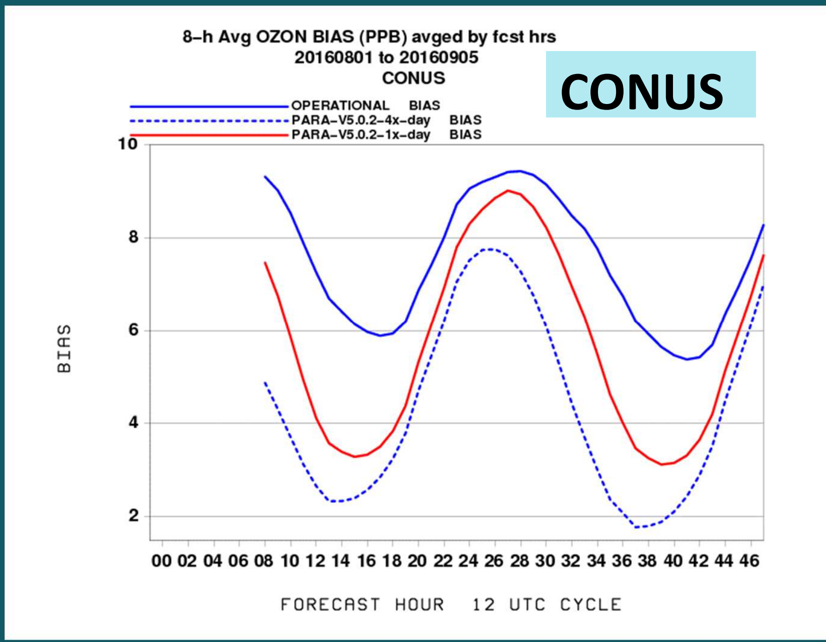
24 h avg $PM_{2.5}$ on June2 2016



Courtesy A. Sleinkofer et al. EMC internship

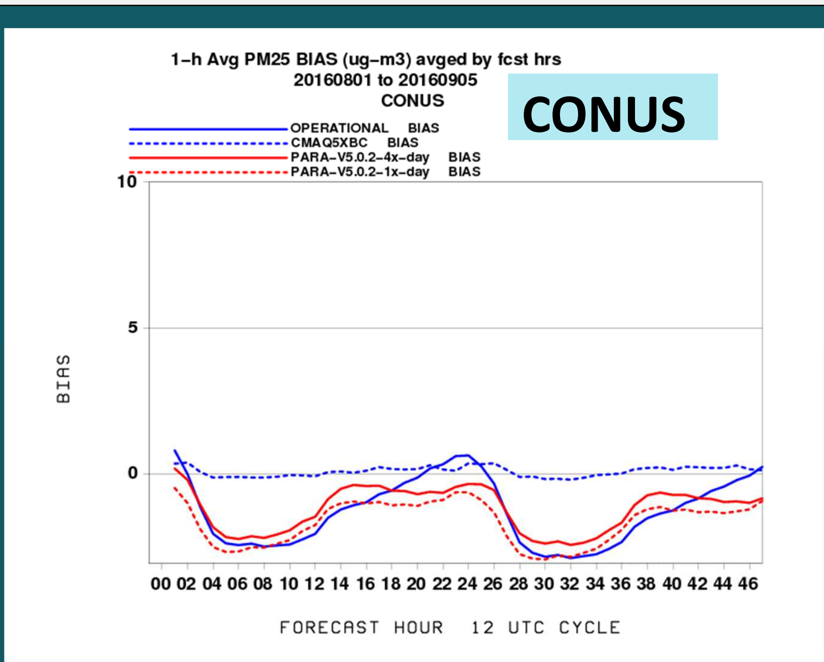
Performance comparison between Prod & CMAQ5.0.2

Bias for MDA8 O_3 8/01-9/15/2016: Prod; CMAQ5.0.2 12Z 1/day; bias correct



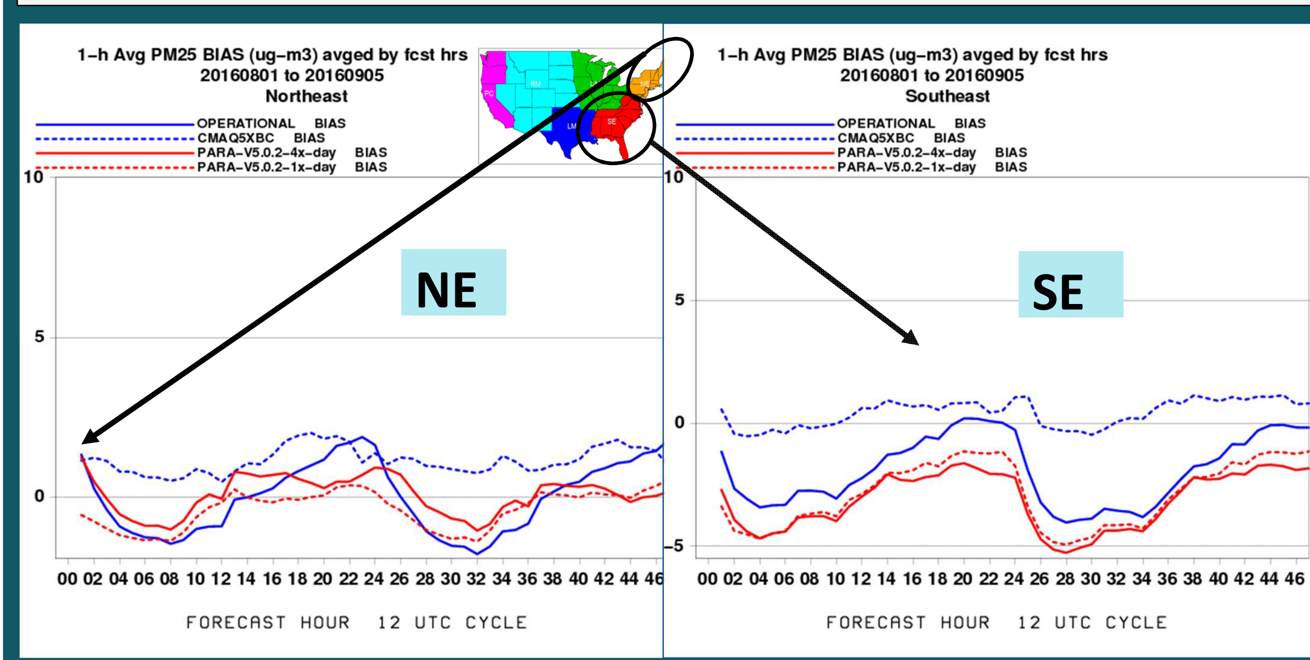
Performance comparison between Prod & CMAQ5.0.2 cont'd

Bias for hourly $PM_{2.5}$ 8/01-9/15/16: Prod; CMAQ5.0.2 12Z 1/day; bias correct



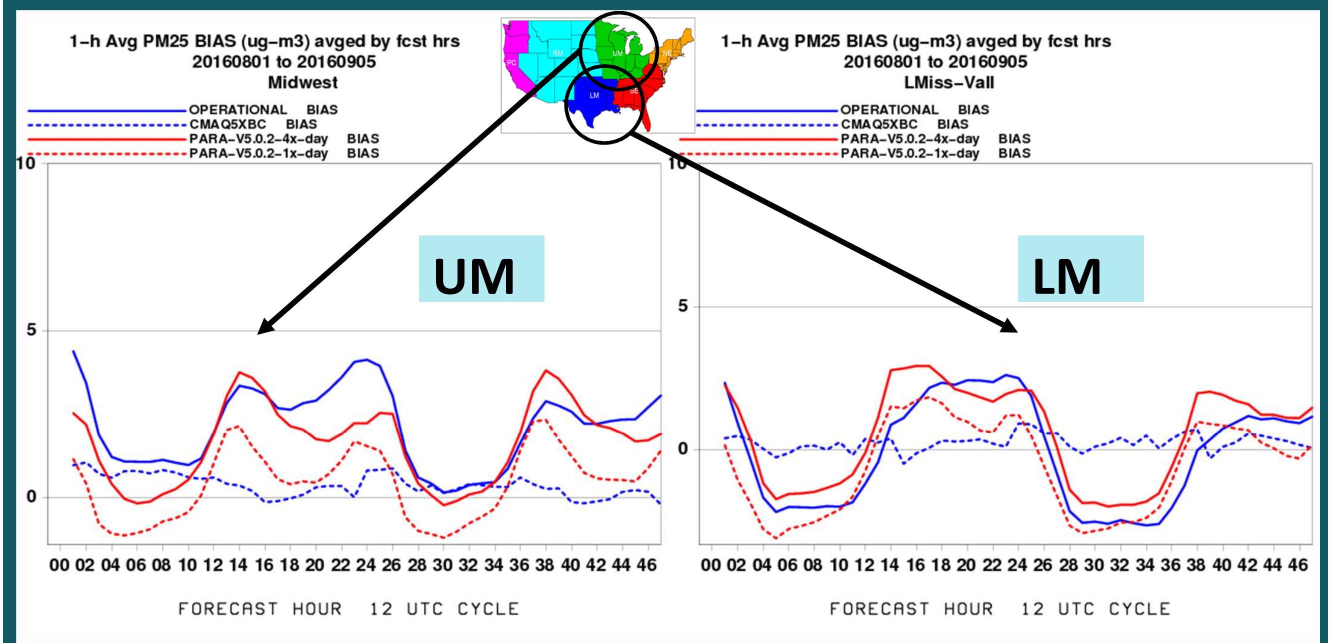
Performance comparison between Prod & CMAQ5.0.2 cont'd

Bias for hourly $PM_{2.5}$ 8/01-9/15/16: Prod; CMAQ5.0.2 12Z 1/day; bias correct



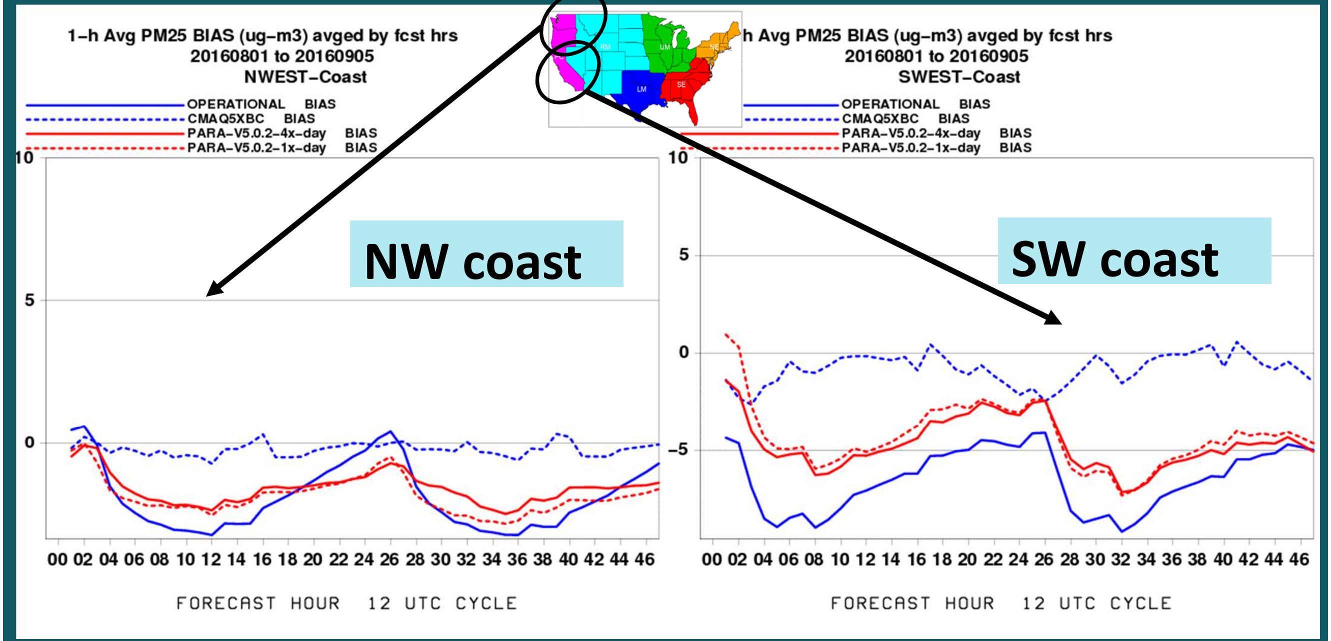
Performance comparison between Prod & CMAQ5.0.2 cont'd

Bias for hourly $PM_{2.5}$ 8/01-9/15/16: Prod; CMAQ5.0.2 12Z 1/day; bias correct



Performance comparison between Prod & CMAQ5.0.2 con'd

Bias for hourly $PM_{2.5}$ 8/01-9/15/16: Prod; CMAQ5.0.2 12Z 1/day; bias correct



ARL Air Resources Laboratory

Conducting research and development in the fields of air quality, atmospheric dispersion, climate, and boundary layer

Evaluation Metrics:

$$N\_Mean\_Bias = \frac{1}{N}\sum_{i=1}^{N}\frac{(P_i - O_i)}{O_i}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y - \bar{y})^2}$$

$$index\_agreement = 1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(|P_i - \overline{O}| + |O_i - \overline{O}|)^2}$$

e.g., Willmott et al., 2011
I.J. Climatology
doi:10.1002/joc.2419

MDA8 O_3 (ppb) performance metrics between Prod and CMAQ5.0.2

Aug 1-Sep 5 2016

Day-1 performance		obs	Bias	Normalized mean bias%	RMSE	Coeff corr, r	Index of agreement
CON	**PROD**	**40.0**	**6.8**	**17.0**	**11.5**	**0.70**	**0.60**
	502		**3.1**	**7.8**	**9.8**	**0.70**	**0.64**
PC	**PROD**	**45.2**	**0.12**	**0.27**	**10.0**	**0.85**	**0.72**
	502		**-1.1**	**-2.4**	**9.9**	**0.85**	**0.72**
RM	**PROD**	**48.0**	**2.1**	**4.9**	**8.7**	**0.70**	**0.60**
	502		**-1.8**	**-3.6**	**8.4**	**0.70**	**0.60**
UM	**PROD**	**36.0**	**9.0**	**25.0**	**11.4**	**0.86**	**0.58**
	502		**4.5**	**12.33**	**8.8**	**0.82**	**0.64**
LM	**PROD**	**34.0**	**11.6**	**33.5**	**14.4**	**0.75**	**0.47**
	502		**9.0**	**26.5**	**13.5**	**0.65**	**0.48**
NE	**PROD**	**40.2**	**9.7**	**31.4**	**12.5**	**0.80**	**0.55**
	502		**3.9**	**15.5**	**8.2**	**0.80**	**0.65**
SE	**PROD**	**33.2**	**10.1**	**30.3**	**12.5**	**0.82**	**0.54**
	502		**6.1**	**18.1**	**9.5**	**0.81**	**0.60**

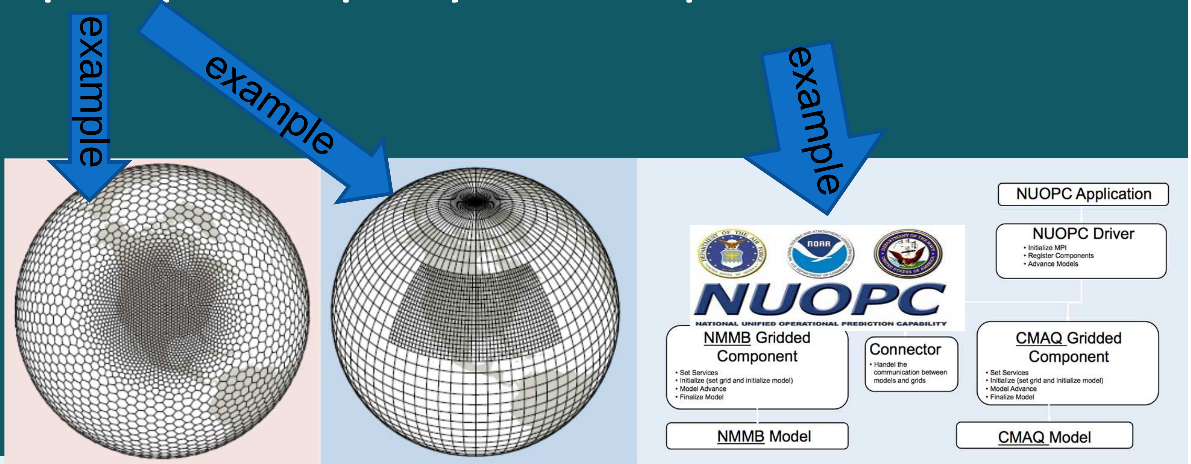
24h avg $PM_{2.5}$ ($\mu g\ m^{-3}$) performance between Prod and CMAQ5.0.2

Aug 1-Sep 5 2016

Day-1 performance		obs	Bias	Normalized mean bias%	RMSE	Coeff corr, r	Index of agreement
CON	**PROD**	**7.3**	**-0.75**	**-10.0**	**7.6**	**0.19**	**0.41**
	502		**-0.80**	**-11.0**	**7.6**	**0.24**	**0.43**
PC	**PROD**	**8.0**	**-3.3**	**-40.0**	**8.3**	**0.23**	**0.44**
	502		**-3.0**	**-38.0**	**8.9**	**0.26**	**0.45**
RM	**PROD**	**7.2**	**-2.4**	**-33.9**	**10.3**	**0.13**	**0.40**
	502		**-2.3**	**-31.3**	**10.3**	**0.22**	**0.43**
UM	**PROD**	**7.0**	**2.6**	**37.7**	**7.5**	**0.33**	**0.43**
	502		**2.1**	**29.3**	**6.5**	**0.39**	**0.44**
LM	**PROD**	**8.2**	**-1.1**	**-12.8**	**5.8**	**0.30**	**0.44**
	502		**-2.0**	**-24.1**	**6.4**	**0.22**	**0.42**
NE	**PROD**	**6.4**	**0.40**	**6.1**	**5.3**	**0.31**	**0.41**
	502		**0.91**	**14.6**	**5.3**	**0.34**	**0.42**
SE	**PROD**	**7.8**	**-0.8**	**-10.6**	**5.5**	**0.36**	**0.47**
	502		**-1.0**	**-13.0**	**5.5**	**0.36**	**0.45**

Future Directions

- Chemical Analysis: homogeneously generated fields over multiple years
- NAQFC in finer resolutions: Chemically, spatially and temporally
- Incorporation of air-surface exchange processes in air chemistry
- Air chemistry as one of NCEP Earth Modeling System Framework components



Summary

- Anticipated FY17 implementation of CMAQ5.0.2

Improves O_3 forecasting skill
- Reduced RMSE → improved spatial & temporal accuracy

This improvement is attributable to NAM and chemistry in CMAQ5.0.2 & the use of the most updated trend to modulate mobile NOx

Improve $PM_{2.5}$ forecasting skill, esp. during the wildfire season
- Reduced under-estimation of $PM_{2.5}$ in the initialization fields by including a 24 h analysis assisted initialization adjustment
- New BlueSky improves fuel and consumption models
- The NGAC-provided dust boundary condition
- Fugitive dust -- crustal elements, are explicit in cmaq5.0.2

Challenges remains beyond FY17:

- Finer resolution
- Evaluation metrics for fine resolution output
- Complex terrains
- Coastal region over-estimation of O_3
- CMAQ I/O operation bottle-neck
- Test and improve NGAC-Smoke derived dynamic BC
- Irregularity of oil and gas emission inventory
- Mobile emission sources modeled by MOVES2014a

附錄九　Investigating Causes of CMAQ Under Predictions of Sea Salt Aerosol in the San Francisco Bay Area

INVESTIGATING CAUSES OF CMAQ UNDER-PREDICTIONS OF SEA SALT AEROSOL IN THE SAN FRANCISCO BAY AREA

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1. INTRODUCTION

To study health impacts, we used CMAQ to make year-round PM2.5 simulations over Central California for 2012. A comparison of the simulated PM2.5 with observations in the San Francisco Bay Area (SFBA) showed under-prediction of PM2.5 during summer, particularly May. This paper presents an analysis of possible causes of the under-prediction and a suggested remedy for the problem.

2. METEOROLOGY MODEL

We used the WRF model to generate the meteorological data input to CMAQ. The WRF model used a triple nested domain (Fig. 1) with 36km-12km-4km grid resolutions. Domain 3 is centered on Central California. The year-round simulations actually cover the 2nd through the 15th for February to November, and the 2nd to the end of the month for January and December. PM2.5 exceedances in the SFBA happen mostly in January and December so we extended the simulation periods for these two months.

3. AIR QUALITY MODEL

For most of the air quality simulations, we used the CMAQ model version 5.0.2 and saprc99-ae5 chemical mechanisms. A few runs were made using CMAQ version 5.1 and saprc07-ae6 chemical mechanisms for comparison purposes. Domain 3 with 4 km grid resolution was used for the majority of the air quality simulations. Lateral boundary conditions for the most model runs were derived from MOZART data. A few runs used the profile boundary conditions (EPA-derived constant profiles for gases and PM) for reasons to be explained later.

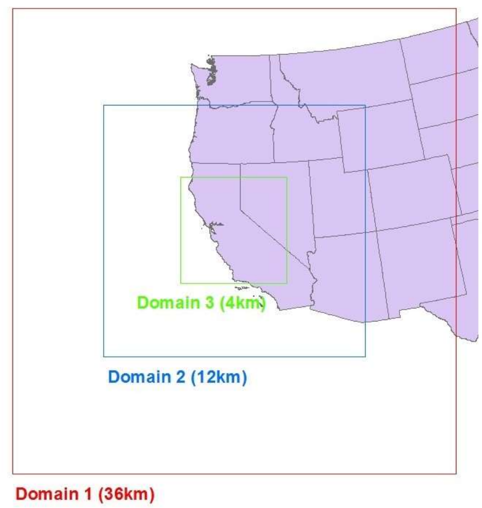

Fig. 1 Triple nested domain used in the WRF simulations.

4. EMISSIONS

We prepared emissions for areas within the jurisdiction of the Bay Area Air Quality Management District (BAAQMD). For areas outside of the SFBA, we used the emissions generated by the California Air Resources Board (CARB).

5. RESULTS OF THE BASE CASE SIMULATION

Fig. 2 shows the daily observed and simulated PM2.5, averaged over all stations in the SFBA. There is a clear pattern of over-prediction of PM2.5 during the winter months and under-prediction during the summer months. The under-prediction is especially noticeable for May, in which the observations showed a systematic gradual increase in PM2.5 from the beginning of the month to the 9th, followed by a gradual decrease in PM2.5 toward the 15th of the month.

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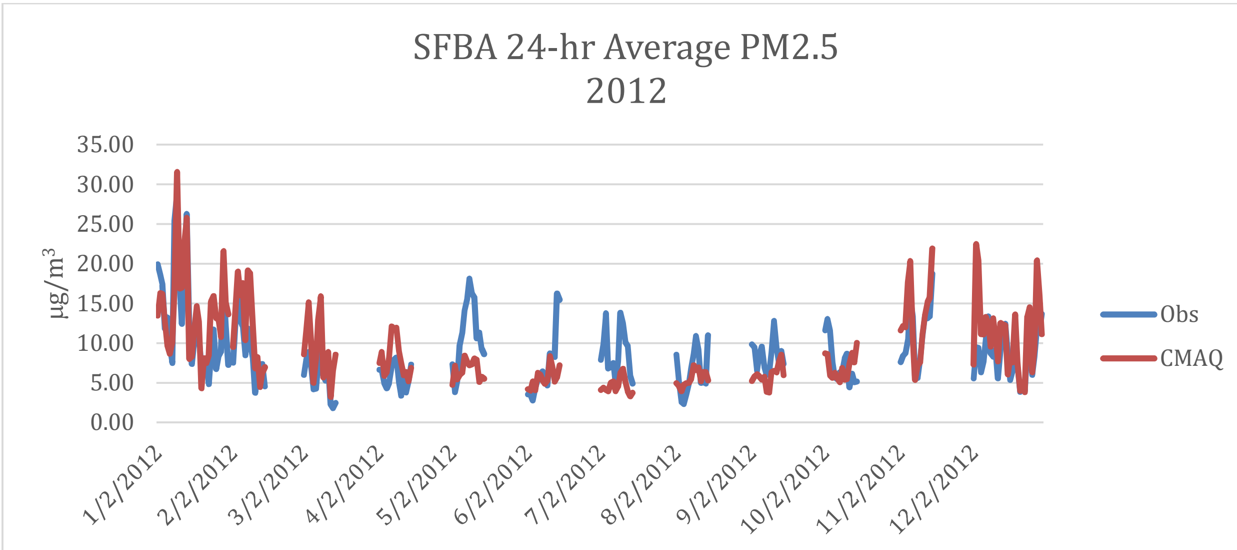

Fig. 2 Daily observed and simulated PM2.5, averaged over all stations in the SFBA.

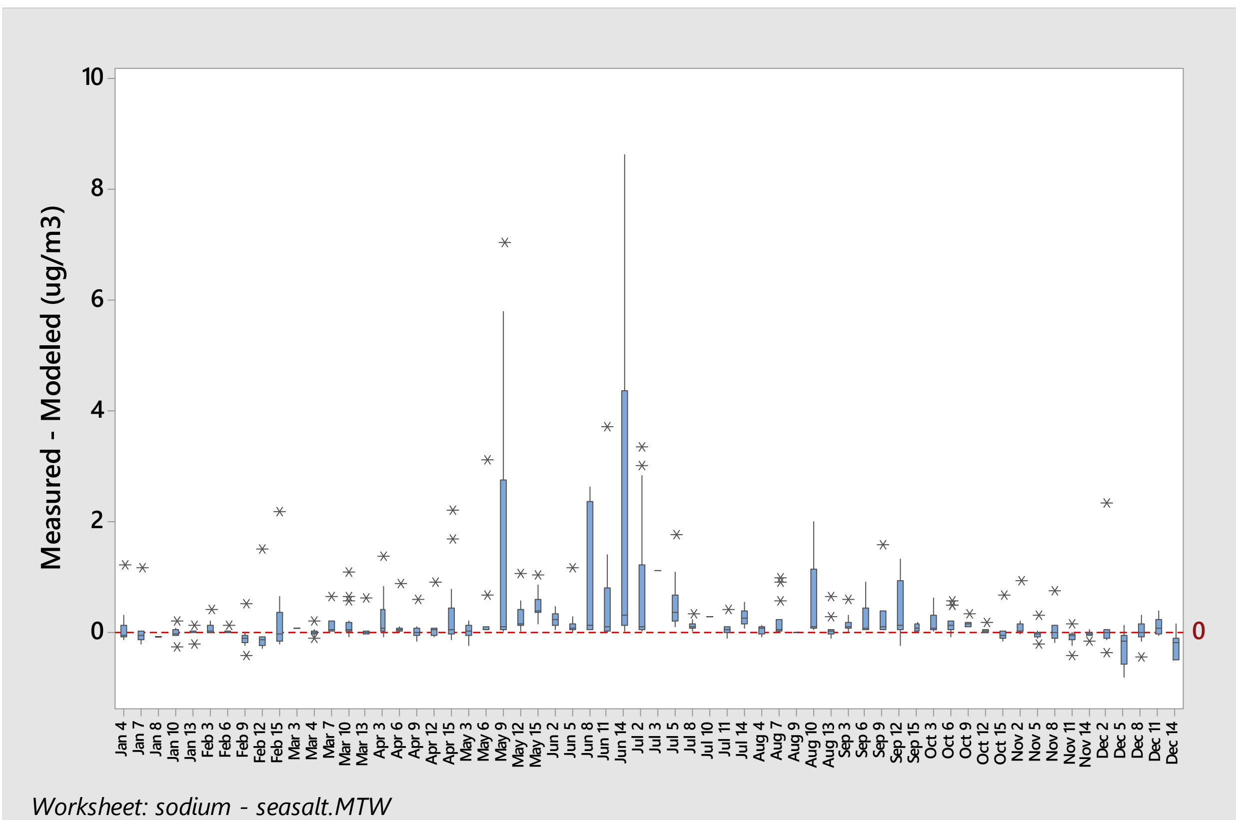

Fig. 3 Daily differences between measured and simulated sea salt averaged over all California stations.

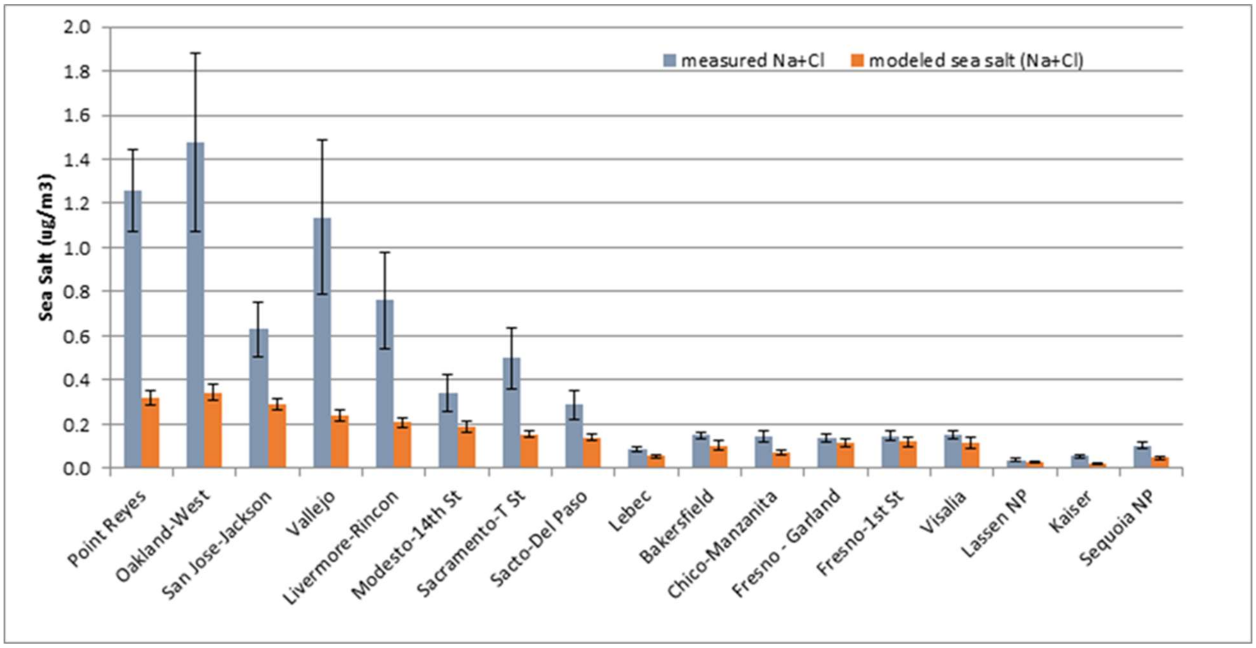

Fig. 4 Observed and simulated annual mean sea salt at selected stations

6. ANALYSIS OF SEA SALT PREDICTIONS

We compared simulated PM2.5 with speciated observation data in order to understand the cause of under-prediction of PM2.5 during summer. Fig. 3 shows boxplots of the daily differences between measured and simulated sea salt averaged over all California stations. The speciated data are available every six days for most stations. For a few stations, the speciated data are available every three days.

During winter months, the observed and simulated sea salts are comparable; however, for many summer days, observed sea salt is considerably larger than the simulated values. For May 9, the day of special emphasis in this paper, 50% of the observed sea salt is 3 $\mu g/m^3$ larger than the simulated values. The observed sea salt at one station is 7 $\mu g/m^3$ larger than the simulated value.

Fig. 4 shows the observed and simulated annual mean sea salt concentration at selected stations. The arrangement of the stations is based on distance from the coast. It is obvious that the stations close to the coast have larger sea salt concentrations. San Jose has less sea salt than Vallejo and Livermore because the path of the prevailing summertime onshore wind crosses Vallejo and Livermore on the way toward the Central Valley instead of passing through San Jose.

The CMAQ model under-predicted sea salt at all stations. The under-prediction is most severe for stations near the coast, which include all stations in the SFBA. The observed annual average sea salt is 2-5 times the simulated values. The problem of under-prediction in the Central Valley is much smaller.

At Point Reyes and West Oakland, the CMAQ model under-predicted the daily average sea salt almost every day (Figs. 5a and 5b). The under-prediction is much larger in the summer than in the other months. The daily observed sea salt can be as large as 10 times the simulated value. It could indicate some difficulty for the sea salt algorithm in CMAQ when applied to California and the eastern Pacific, where the wind during summer is particularly strong due to the intense Pacific high.

In Fig. 5, the simulated sea salt does not change significantly from summer to winter while the observed sea salt has maxima in May and June. Also, sea salt at West Oakland has much larger summer-winter differences than at Point Reyes. This is understandable since Point Reyes is right by the ocean and is affected by the ocean-generated sea salt year round. West Oakland is on the east side of San Francisco Bay, and the observed sea salt at this location is governed by the prevailing wind as much as the ocean-generated sea salt. During May and June, the onshore wind is particularly strong and it can easily transport ocean sea salt to this station. During winter months, offshore wind prevails and West Oakland has much less ocean sea salt.

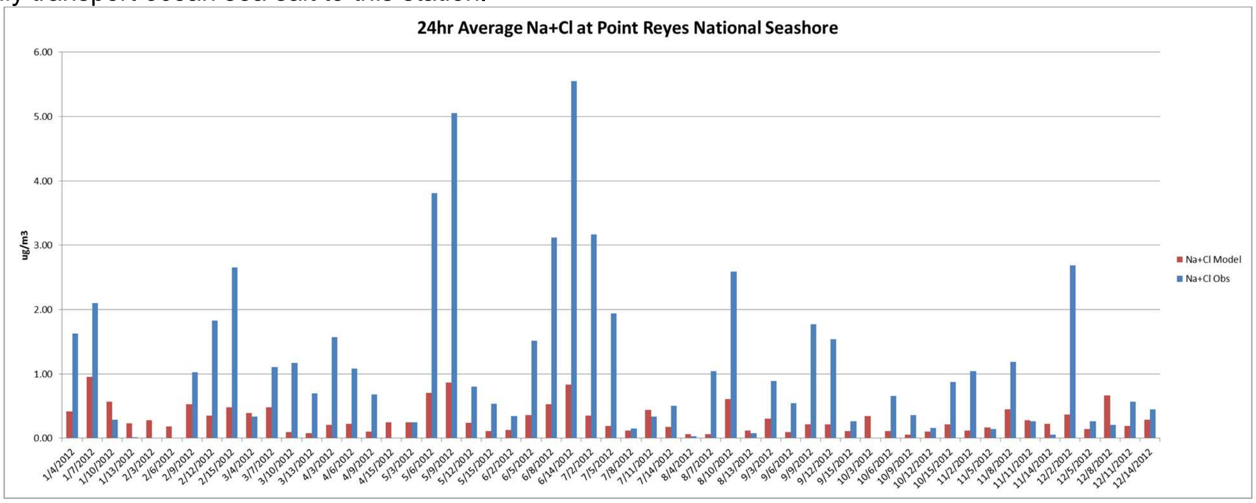

Fig. 5a Daily average sea salt at Point Reyes station

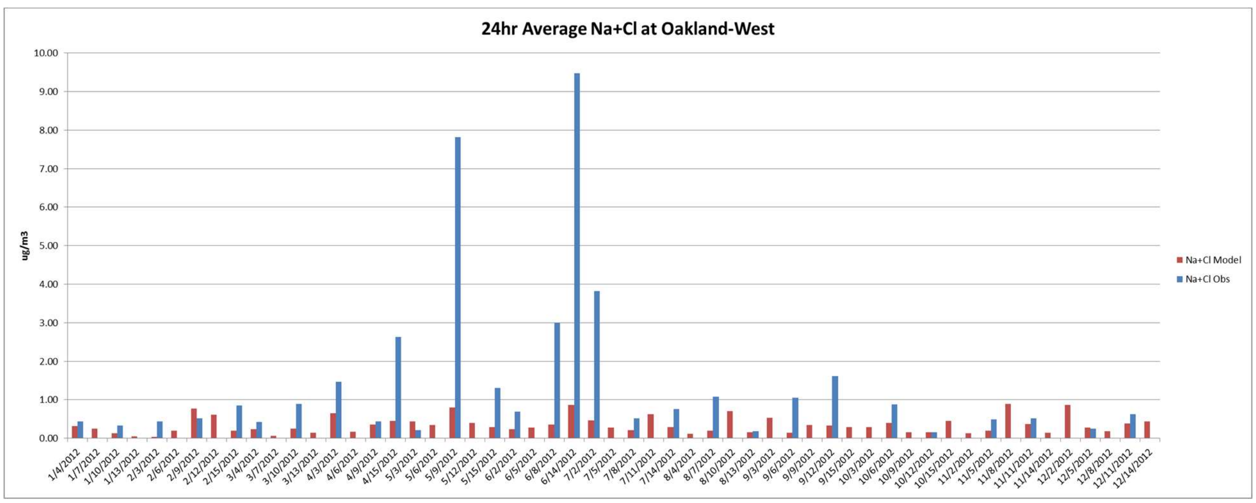

Fig. 5b Daily average sea salt at West Oakland station

7. SEA SALT GENERATION

Domain 3, over which most of our simulations were made, covers a limited ocean area. In order to understand the generation of sea salt in CMAQ, we did a few runs using domain 1, which extends 1000 miles over the Pacific Ocean from the California coast. For these runs, we set anthropogenic emissions to zero in the areas outside of domain 3. We also used the profile lateral boundary conditions. These assumptions should not cause a problem for the purpose of studying sea salt generation over the ocean.

An example of the WRF-simulated winds on May 9 is shown in Fig. 6. This is the day with high observed sea salt in the SFBA. The wind is especially strong over the ocean, from the northern California coast to the southwestern model boundary. This is apparently a high sea salt generation area.

The concurrent sea salt concentrations are shown in Fig. 7. The area of maximum sea salt is several hundred km south of the area of strong wind and it is the area of sea salt accumulation. The simulated maximum sea salt is located by the coast south of the SFBA and has a magnitude of 2.3 $\mu g/m^3$. This value is much less than the daily average sea salt on May 9 at either Point Reyes or West Oakland (Fig. 5). We can also see sea salt intrusion into the SFBA in Fig. 7. The concentration, though, is less than 1 $\mu g/m^3$.

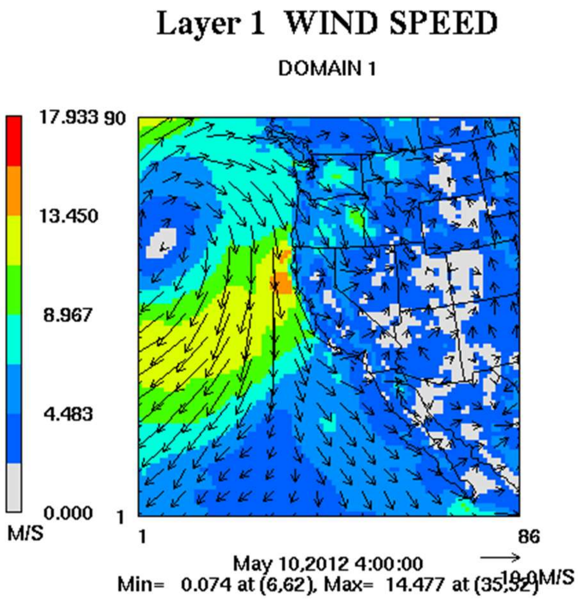

Fig. 6 The WRF model simulated wind speed and wind vector on domain 1.

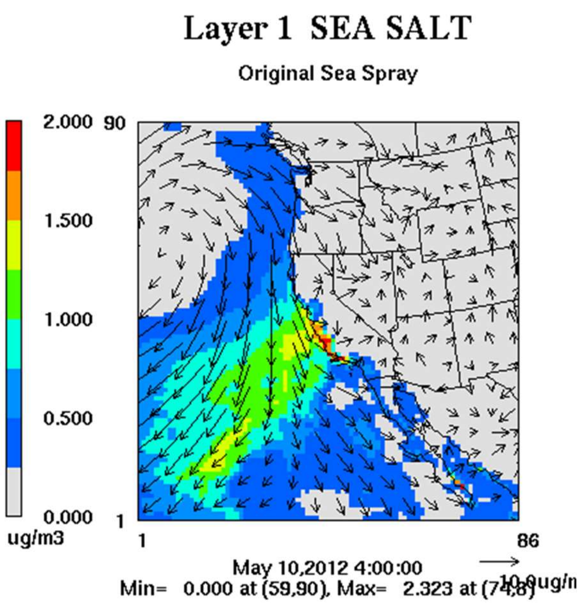

Fig. 7 The CMAQ simulated sea salt (with wind vector) on domain 1.

These results clearly show the under-prediction of sea salt by CMAQ. The magnitude of under-prediction ranges from a factor of 2 to a factor of 10. As a test, we increased the sea salt emission rate in the CMAQ model by a factor of 4 (Fig. 8). The patterns of sea salt, shown in Figs. 7 and 8, remain very similar (note an increase of 4 in the color scale in Fig. 8). The increase in sea salt emission by a factor of 4 actually increased the concentration of sea salt more than 4 times.

Figure 9 shows sea salt concentrations in domain 3 after sea salt emissions were increased by a factor of 4. We can clearly see the sea salt intrusion into the SFBA and the California Central Valley. Now, sea salt concentrations around San Francisco Bay are between 5 and 6 $\mu g/m^3$, much closer to the observations.

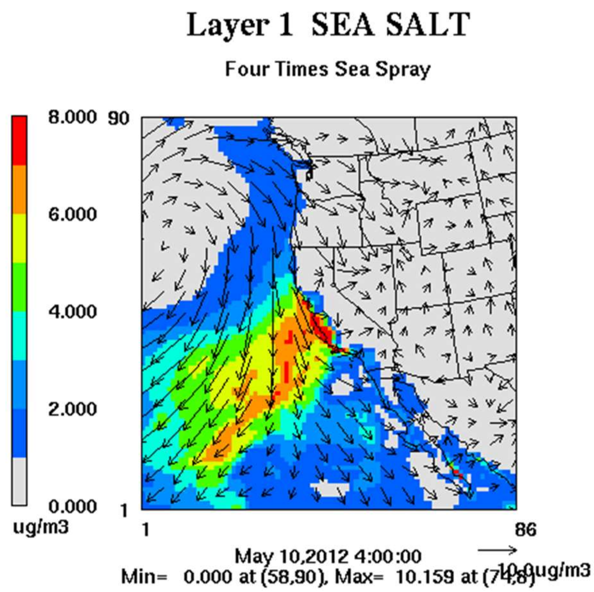

Fig. 8 The CMAQ simulated sea salt (with wind vector) on domain 1 using 4 times the sea salt emission rate.

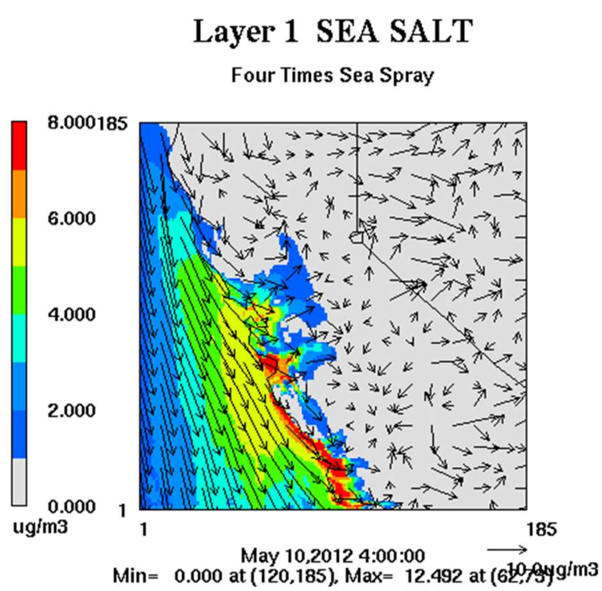

Fig. 9 The CMAQ simulated sea salt (with wind vector) on domain 3 using 4 times the sea salt emission rate.

Figure 10 shows a comparison of daily sea salt simulated with CMAQv5.0.2 to corresponding observations, both averaged over West Oakland, Vallejo and Livermore (observation data are only available for May 3, 9, and 15). Even with 4 times increased the sea salt emission rate, CMAQ version 5.0.2 still under-predicted sea salt by 30% on May 9, the day with high observed sea salt. On the two low sea salt days, it over-predicted sea salt on May 3 and under-predicted sea salt on May 15.

8. SEA SALT ENHANCEMENT IN CMAQv5.1

CMAQ version 5.1 was released after most of our experiments were finished. This version includes a revision that shifts some coarse mode sea salt to the accumulation mode. While experimenting with CMAQv5.1, we encountered a severe lateral boundary problem for PM. Large PM values, much larger than the values specified at the lateral boundary by MOZART data, periodically enter from the western boundary and greatly affect simulated PM2.5 in the SFBA. The model does give reasonable results using profile boundary conditions, which are relatively clean of PM.

Using profile boundary conditions, we proceeded to test the new version. Daily sea salt, simulated using CMAQv5.1 with the factor-of-4 increase in sea spray, is also shown in Fig. 10. Version 5.1 greatly improved sea salt predictions on all three days with observations. On May 9, the day with the largest observed sea salt, the simulation result is almost perfect.

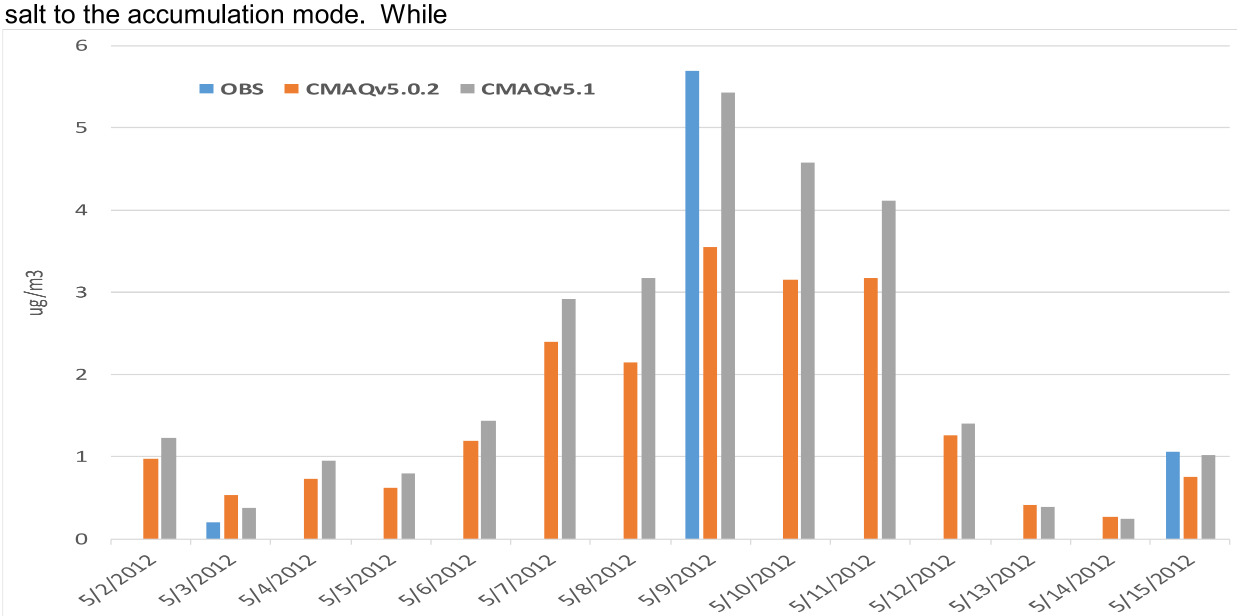

Fig. 10 Simulated sea salt with 4 times sea spray averaged over West Oakland, Vallejo and Livermore.

9. CONCLUDING REMARKS

We made year-round PM2.5 simulations for 2012 using CMAQv5.0.2 and found under-prediction of PM2.5 during the summer months. This under-prediction can be traced to the under-prediction of sea salt. An increase in sea salt emissions by a factor of 4 in the CMAQ model greatly improved the simulated sea salt. A simulation using CMAQv5.1, again with 4 times sea salt emissions, yielded simulated sea salt that almost matched observed sea salt in the SFBA.

We found problems with the lateral boundary treatment of PM species in the western and northern boundaries, i.e. the inflow boundaries. This problem created periodic unreasonably large inflows of PM into the domain and prevented us from using MOZART boundary conditions for the CMAQv5.1 runs.

For future work, we plan to collaborate with CMAQ model developers to refine sea salt emission rates and to resolve the problem in the lateral boundary treatment of PM species in CMAQv5.1.