Highlights of Community Modeling and Analysis System (CMAS) 2010 Conference

Jim Smith & Ron Thomas,
Air Quality Division

Presented to Southeast Texas Photochemical Modeling Technical Committee

December 16, 2010

CMAS 2010

- Although primarily focused on the Community Model for Air Quality (CMAQ), the CMAS conference offers much for all photochemical modelers.
- The majority of papers are directly relevant to regulatory modeling applications.
- 78 technical presentations and 62 posters.
- Presenters from several countries, EPA, private industry, states, and universities.

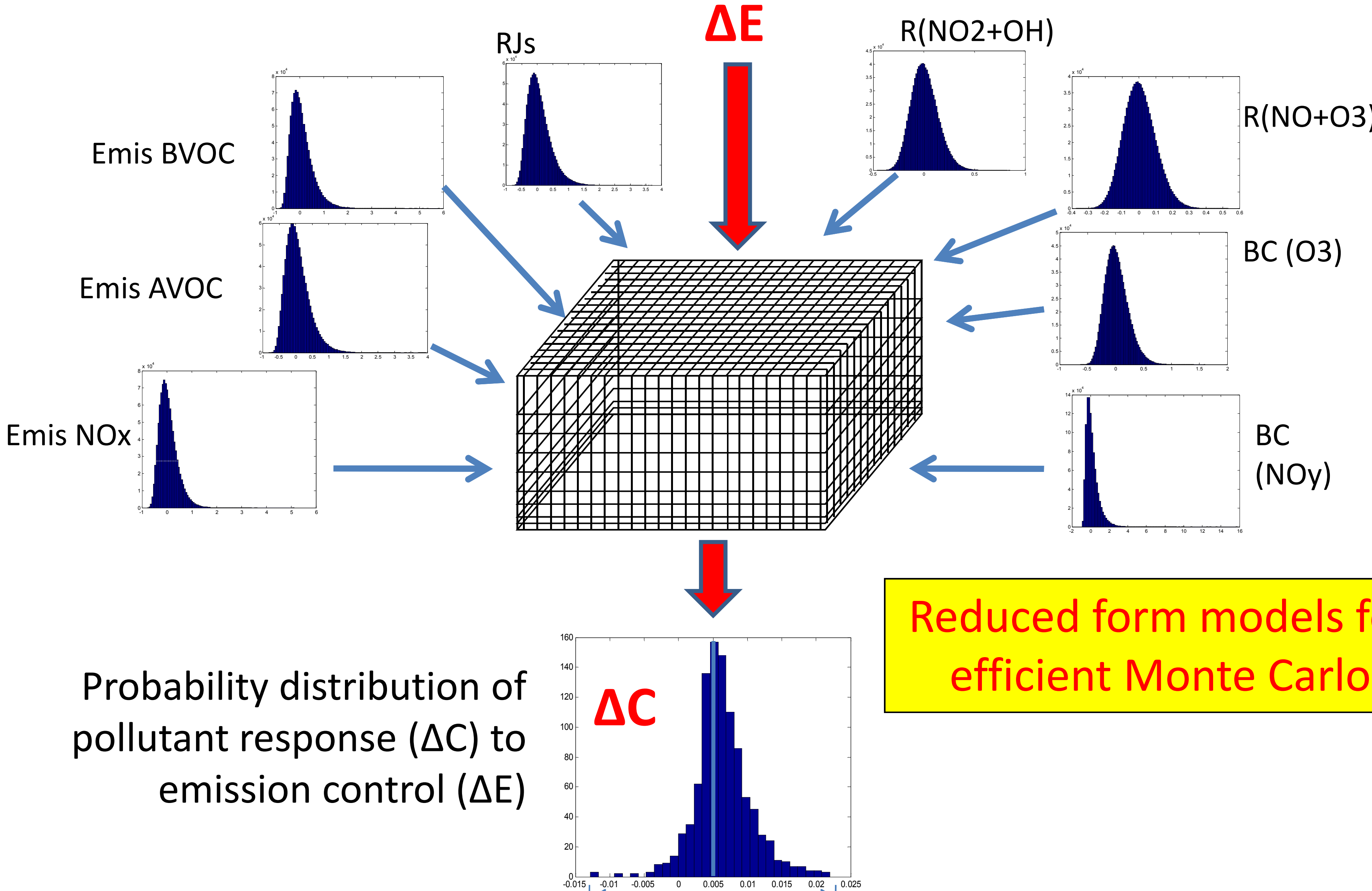
Notable Papers

Uncertainties Influencing Health-based Prioritization Of Ozone Abatement Options

Daniel S. Cohan, Antara Digar & Wei Tang, Rice University
Michelle L. Bell, Yale University

- Studied uncertainty in health benefit estimates as a function of parametric uncertainties in Air Quality model inputs and concentration-response (C-R) function.
- Used a reduced-form model to characterize parametric model uncertainties.
- Uncertainties in AQ model leading drivers of uncertainty in benefits estimation
- Urban NO_X emissions tend to have larger and more uncertain health impacts.

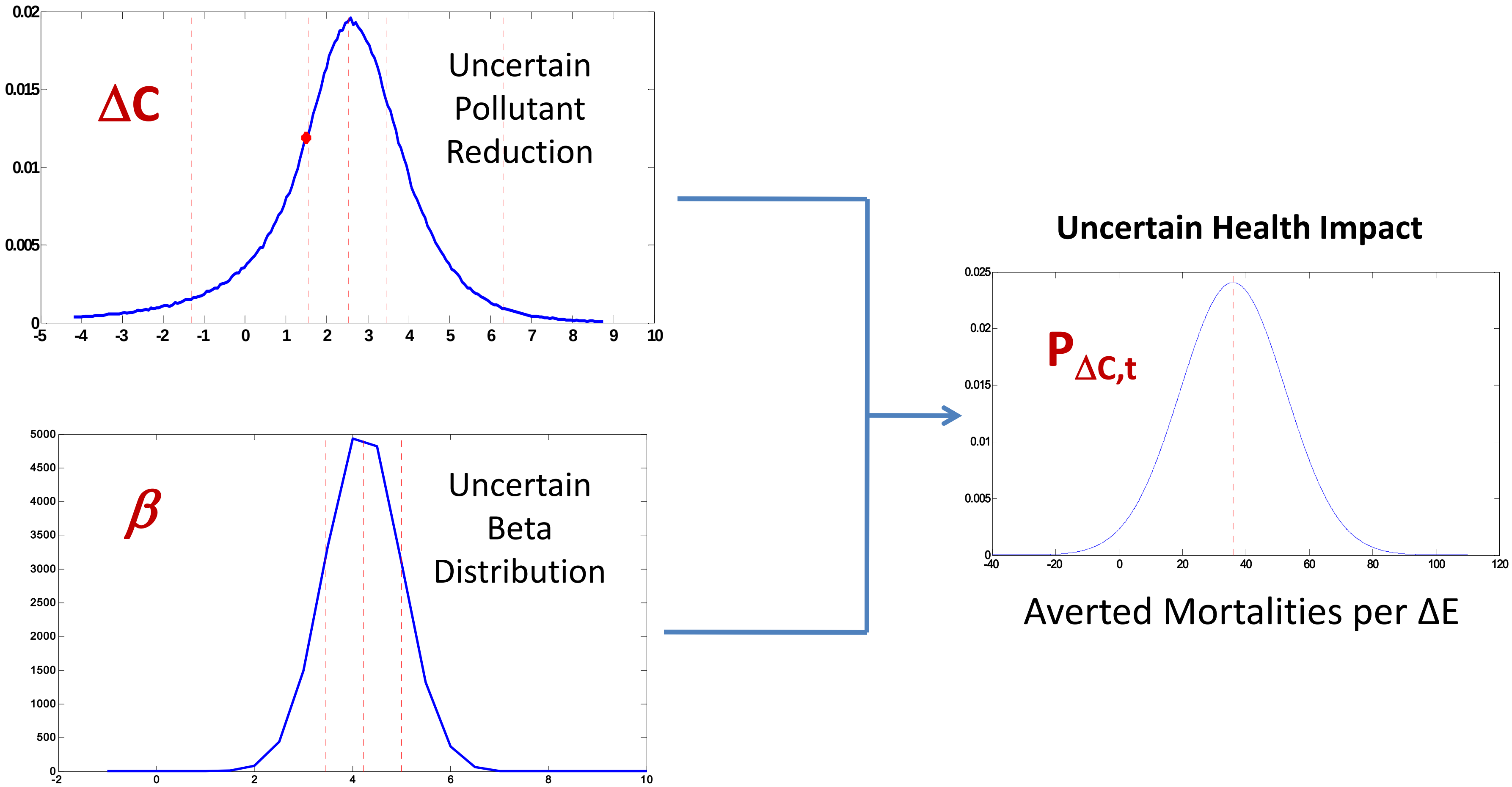
Parametric Uncertainty of Sensitivities



Probability distribution of pollutant response (ΔC) to emission control (ΔE)

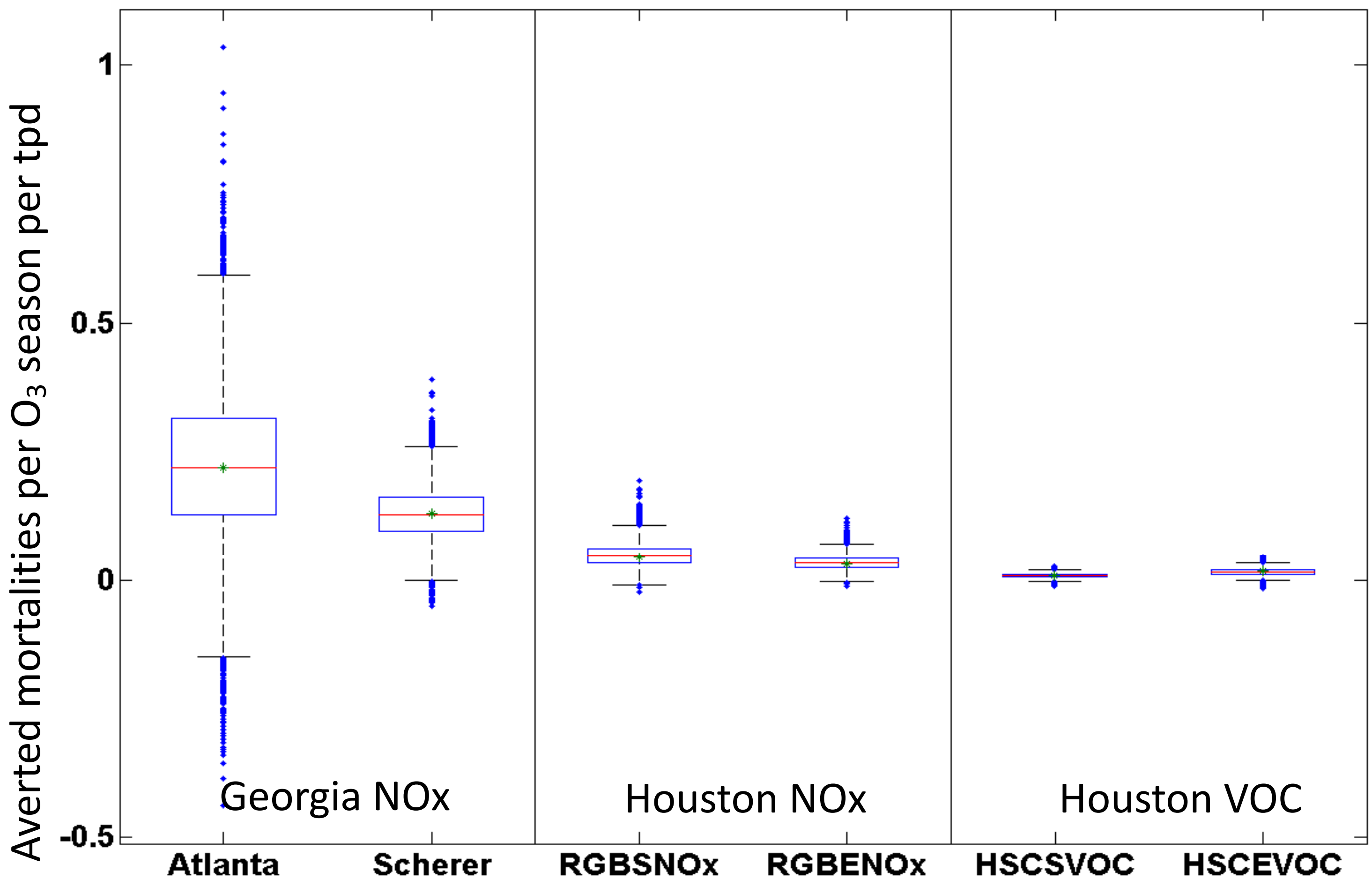
Reduced form models for efficient Monte Carlo

Linking Uncertain Sensitivities and C-R Functions



Uncertain health impact due to uncertain ozone impact (ΔC) and C-R function (β)

Uncertainty Of Health Benefits



- **Uncertainties are large relative to median impacts**
- **Outliers driven by uncertainty in E_{NOx}, E_{bioVOC}, and photolysis rates**

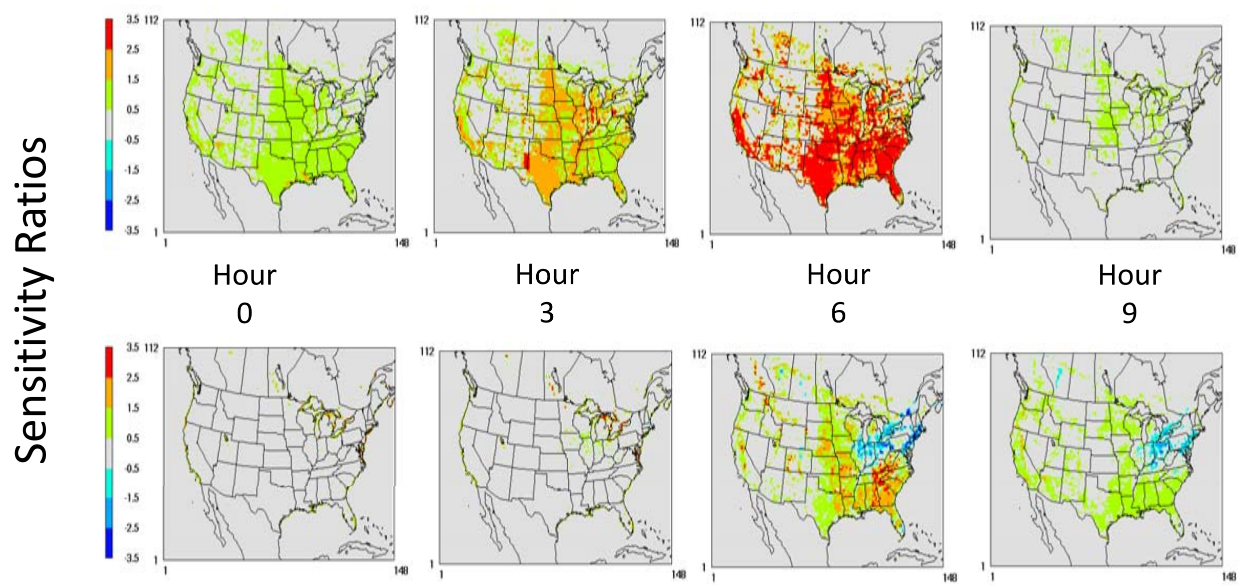
(Results based on 8-hour metric, with uncertain ϕ and β)

Temporal Source Apportionment of Policy-Relevant Air Quality Metrics

Nicole MacDonald & Amir Hakami, Carelton University

- Used CMAQ-Adjoint to relate modeled ozone concentrations to emissions as a function of time.

Time Evolution of SRs



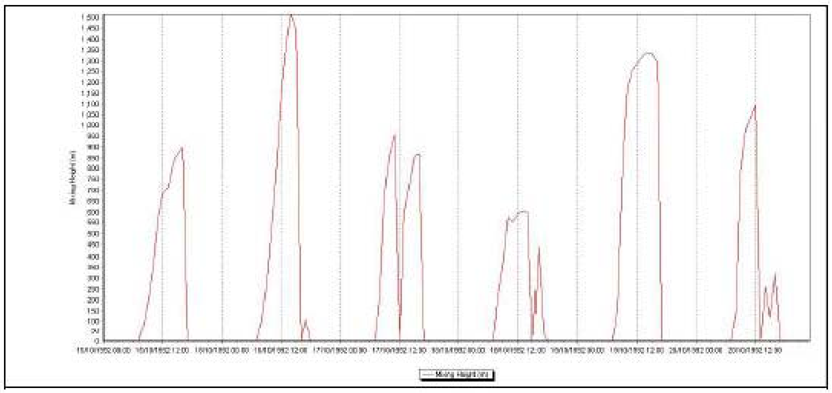
Proof-of-Concept Evaluation of Use of Photochemical Grid Model Source Apportionment Techniques for Prevention of Significant Deterioration of Air Quality Analysis Requirements

Bret Anderson, USFS; Kirk Baker & Erik Snyder, USEPA; Ralph Morris & Chris Emery, Environ; Andy Hawkins, State of Kansas

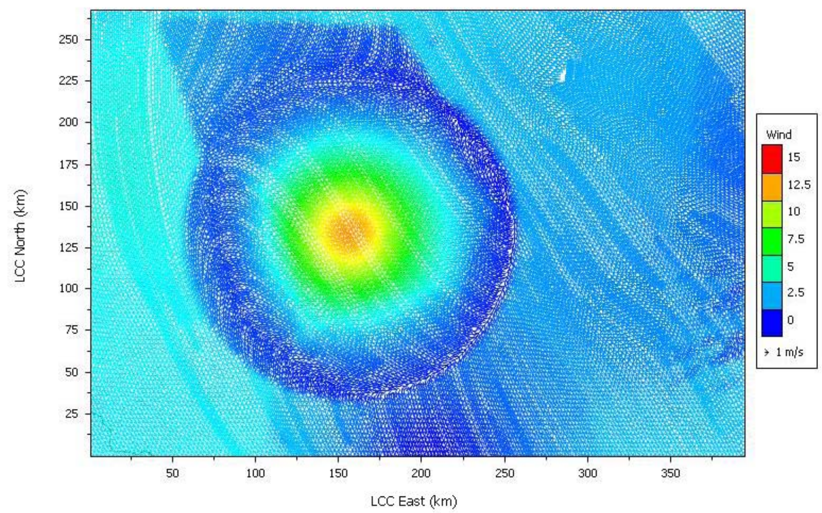
- Explored using a photochemical grid model (CAMx) with source apportionment for PSD permit applications instead of the guideline CalPuff/CalMet system.
- PGMs employ much better science, but are also much more resource-intensive.

Issues with CALMET Meteorology

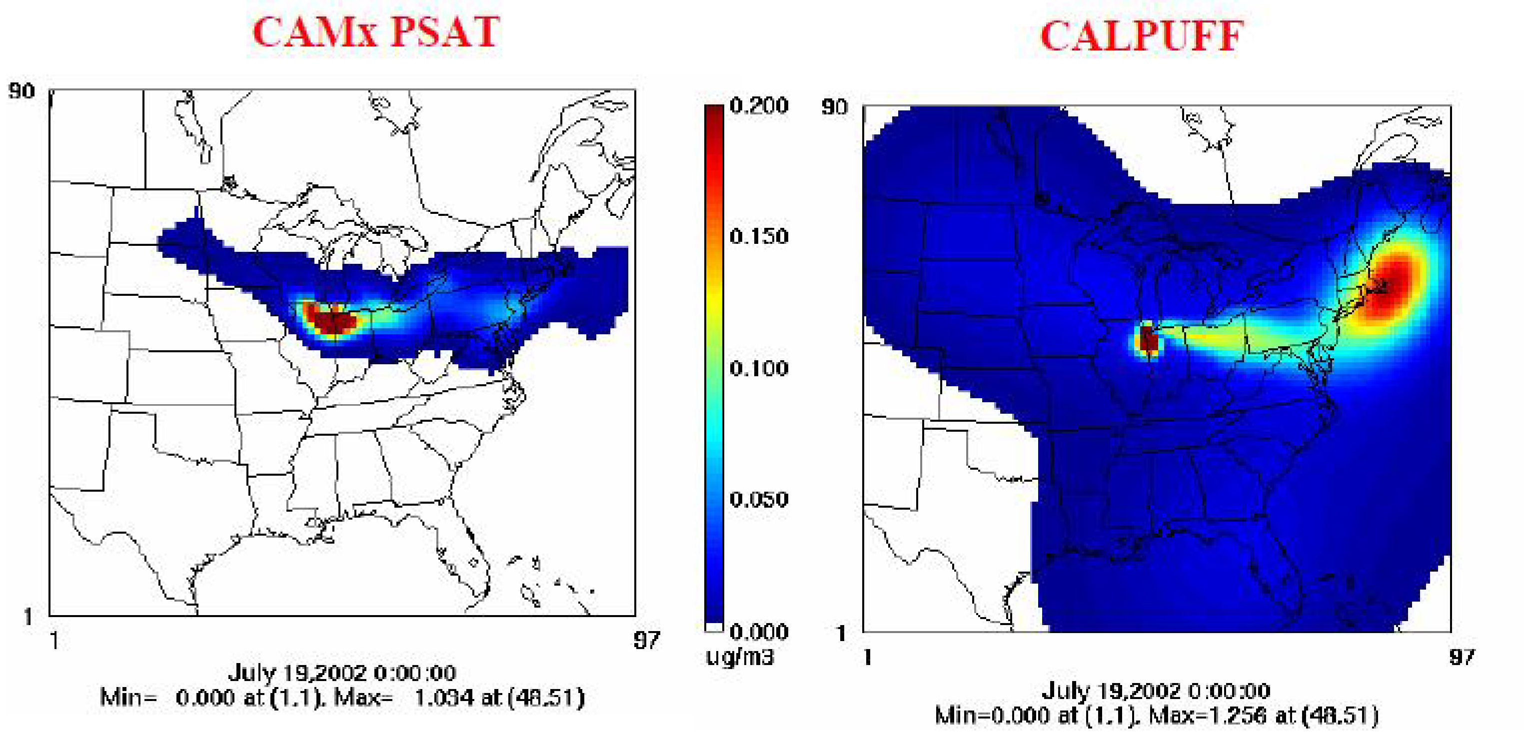
Collapsing CBL's



Objective Analysis Errors



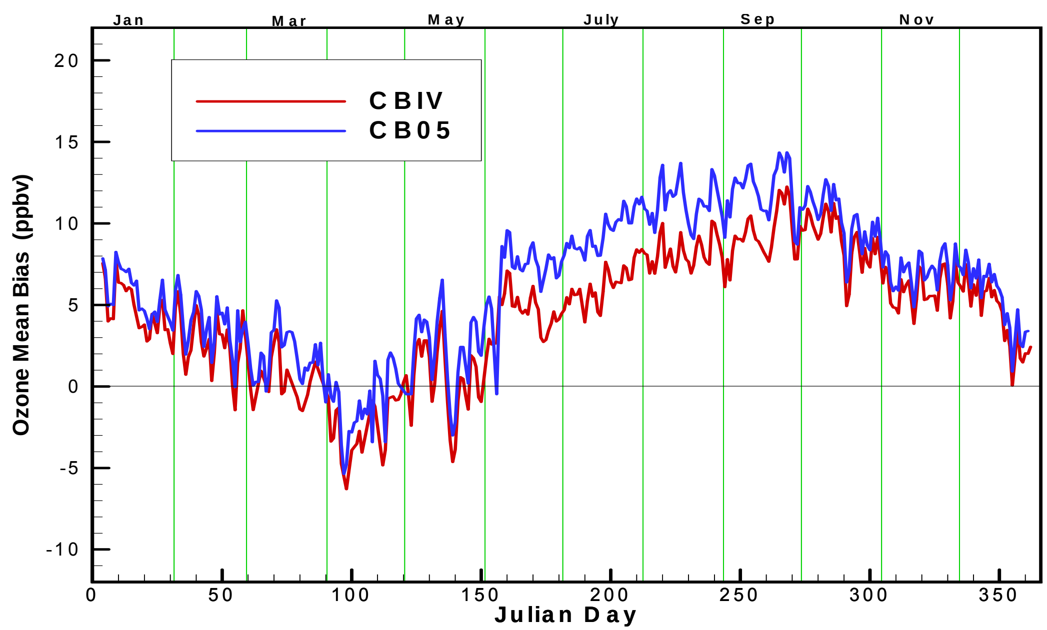
Issues with CALPUFF Chemistry



Investigating Differences in O_3 Production from CB05 and CBMIV Versions of the NAQFC

Rick Saylor, Hsin-Mu Lin, Pius Lee, Binyu Wang, Tianfeng Chai,
Ariel Stein, Daniel Tong, Hyun-Cheol Kim, Yunsoo Choi,
Fantine Ngan, Daewon Byun, NOAA

- Running the National Air Quality Forecast Center model with CB05 produces higher ozone concentrations than using CB-IV.
- Several differences between mechanisms, but largest portion of ozone differential is due to nitrate recycling in CB-05.



Evaluation of the Simulated Planetary Boundary Layer in Eastern Texas

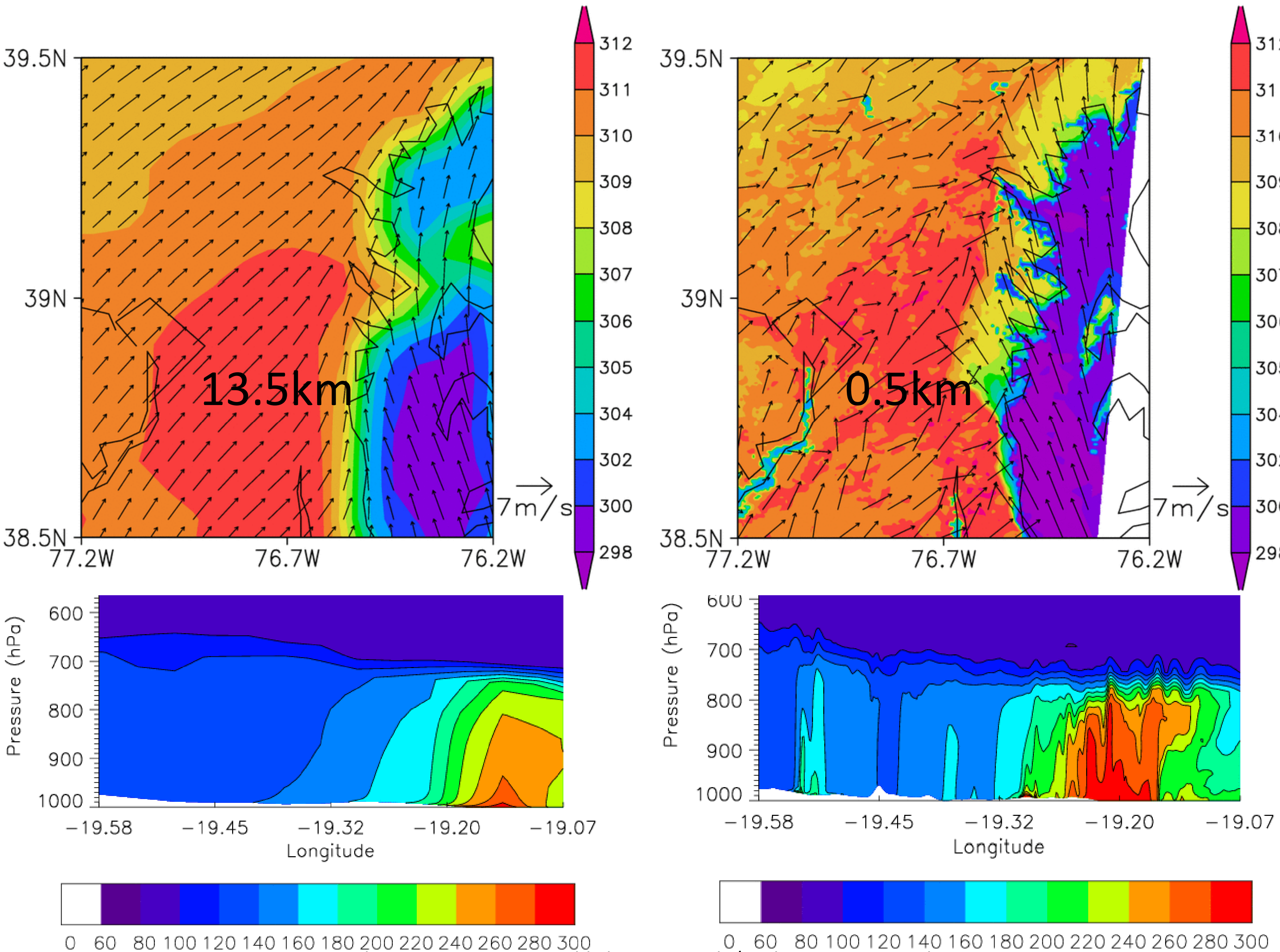
Jenna Kolling UNC), Jonathan Pleim (USEPA), William Vizuete (UNC), Harvey Jeffries (UNC)

- Compared East Texas median hourly PBL values (Aug 13 – Oct. 11, 2006) simulated with WRF/ACM2 with those simulated using MM5/Eta.
- The two methods produced comparable predicted PBL values at three coastal sites, but MM5/Eta tended to produce PBL depths that were too low inland; WRF/ACM2 appears to produce more accurate PBL depths at these inland sites.

How sensitive are trace gas concentrations to the method used to parameterize clouds within CMAQ?

Christopher P. Loughner, Dale J. Allen, Russell R. Dickerson, Da-Lin Zhang, & Kenneth E. Pickering, University of Maryland; Yi-Xuan Shou, China Meteorological Administration

- Most interesting results were obtained through high-resolution (0.5 km) simulations.
- Higher resolution simulations result in a stronger bay breeze.
- A stronger bay breeze prevents pollutants from being transported near the surface from land to water resulting in lower near surface ozone concentrations over the water and higher ozone concentrations near the bay breeze convergence zone.


39.5N
39N
38.5N
77.2W
76.7W
76.2W
13.5km
0.5km
7m/s
312
311
310
309
308
307
306
305
304
302
300
298
Pressure (hPa)
600
700
800
900
1000
−19.58
−19.45
−19.32
−19.20
−19.07
Longitude
0 60 80 100 120 140 160 180 200 220 240 260 280 300
ppb

Impact of Ozone-Alkene Reactions on Formaldehyde Mixing Ratios during the Texas Air Quality Study 2006

Beata Czader, Bernhard Rappenglück, Daewon W. Byun, Soontae Kim, Fong Ngan, University of Houston

- Used CMAQ process analysis to study pathways for nighttime Formaldehyde formation during TexAQS II.
- Up to 5 ppbv of formaldehyse may be formed during the course of the night.
- Ozone-alkene reactions are most important to nighttime formaldehyde production, but NO-methylperoxy radical reactions also important.

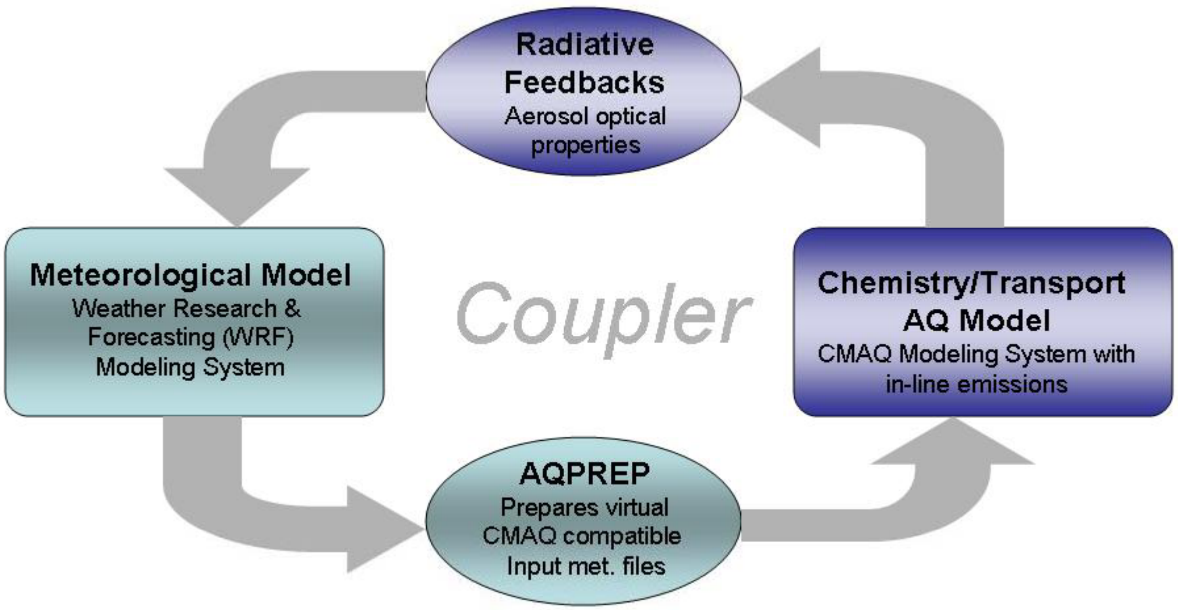
The Community Multiscale Air Quality (CMAQ) Modeling System: Ongoing and Planned Developments

Rohit Mathur, EPA/AMAD

- CMAQv4.7, June 2008
- CMAQv4.7.1, June 2010
- CAMQv5.0, Fall 2011
- SAPR07TB (toxics version B) – more explicit compounds
- Updated CB05 toluene mechanism, Whitten (2010)
- Improved photolysis, albedo
- Organic carbon for more SOA
- Improved PM, aerosol, and fugitive dust
- Improved aqueous chemistry, dry deposition
- MEGAN-based biogenic emissions, lightning NOx

Two-Way Coupled WRF-CMAQ Modeling System

Design and Model Features



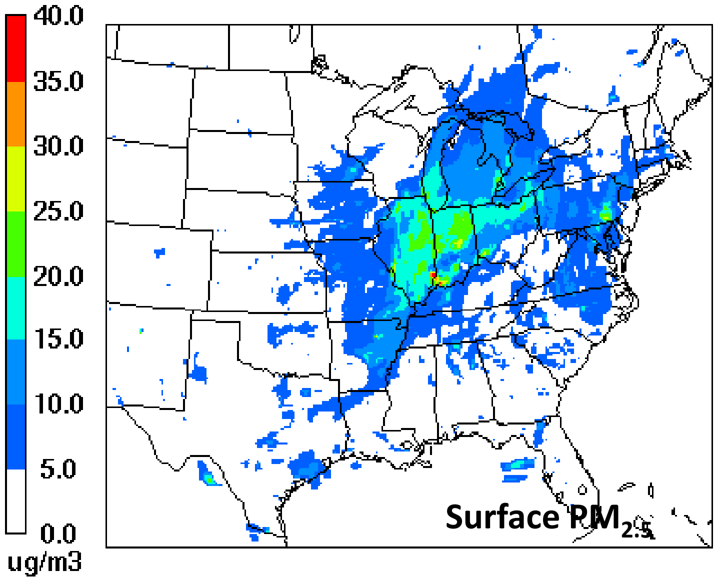
Aerosol Optics & Feedbacks

- Volume weighted refractive indices for 19 wavelength intervals based on
  - Composition and size distribution
  - SO_4^{2-}, NO_3^-, NH_4^+, Na^+, Cl^-, EC, POA, anthropogenic and biogenic SOA, other primary, water
- CAM and RRTMG Shortwave radiation schemes inWRF
- Effects of aerosol scattering and absorption on photolysis
- Effects of O_3 on long-wave radiation
- Indirect effects (**see presentation by S. Yu**)

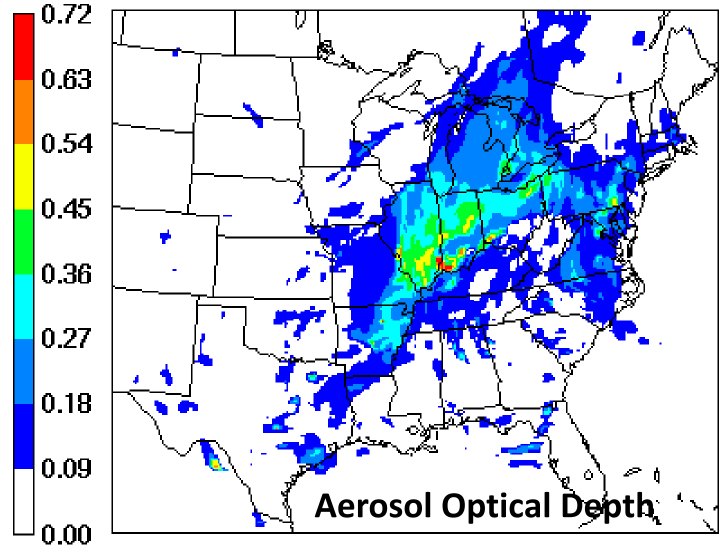
Flexible **design of model coupling allows**

- data exchange through memory resident buffer-files
- flexibility in frequency of coupling
- identical on-line and off-line computational paradigms with minimal code changes
- both WRF and CMAQ models to evolve independently;
  ➡ *Maintains integrity of WRF and CMAQ*

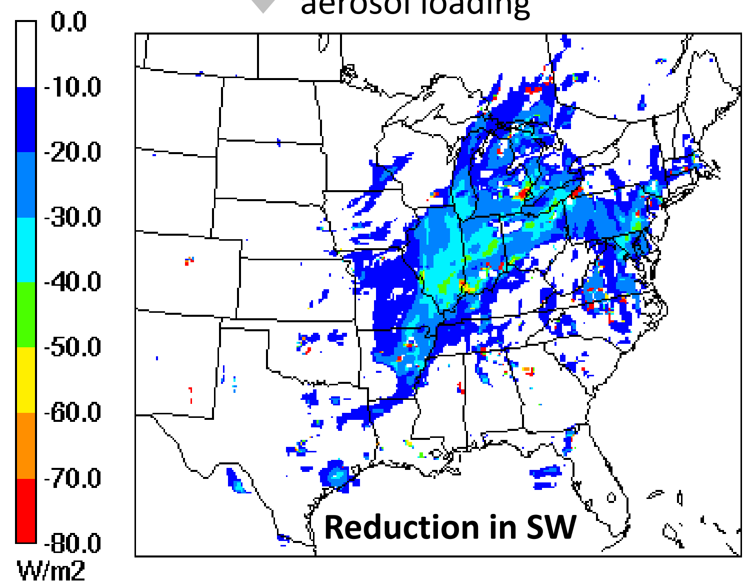
2-Way Coupled WRF-CMAQ Modeling System: Early Results (8/6/06: 22Z)



Optical properties of aerosols

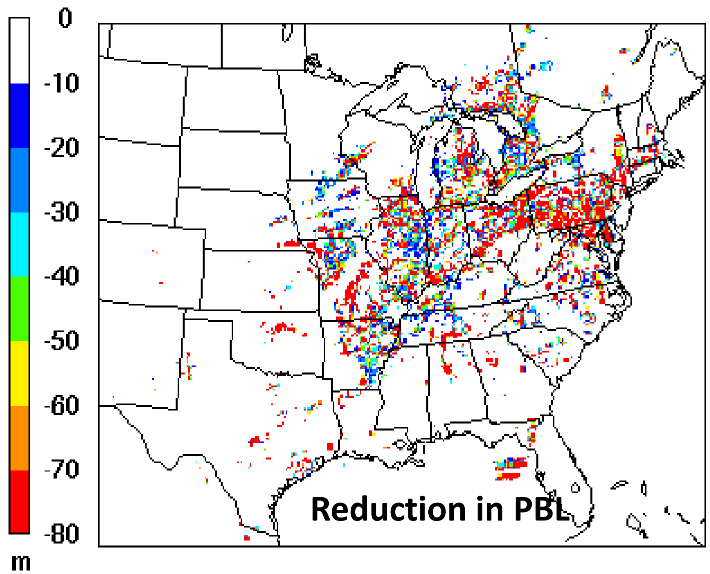


Reduction in shortwave radiation reaching the surface in regions of aerosol loading



Changes in radiation impact simulated dynamical features

(also a reduction In temperature)

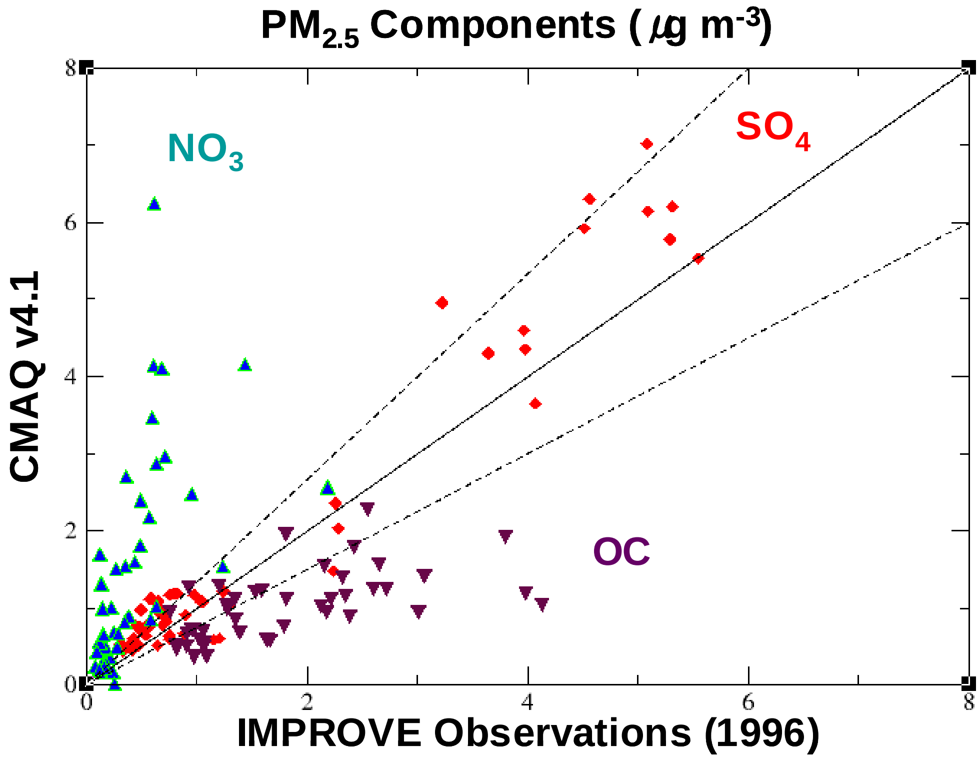


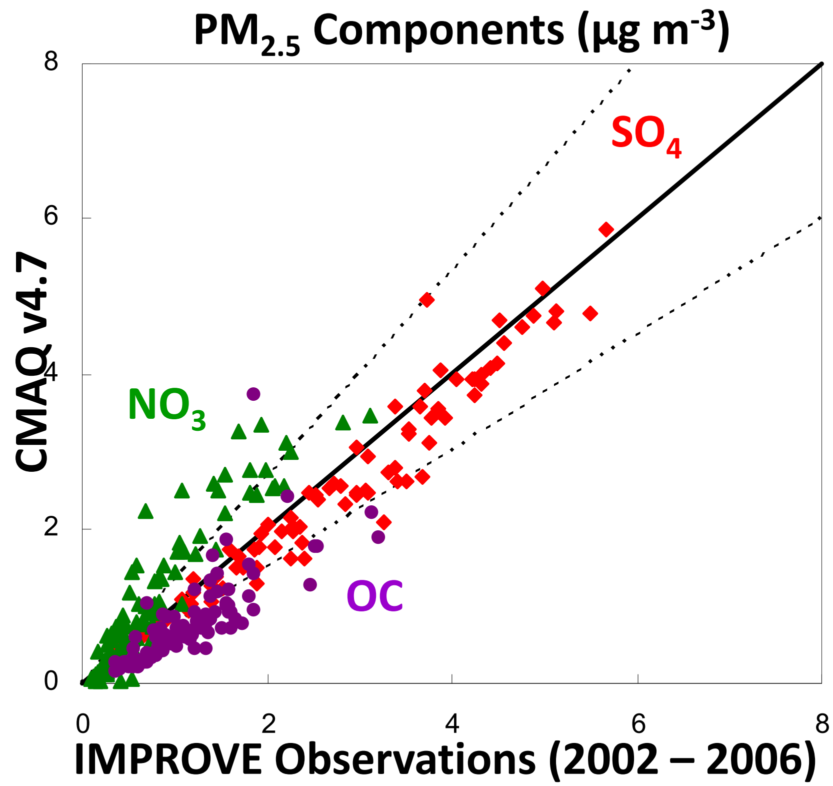
Simulating the Annual-Average PM2.5 Mass Concentrations and Composition Using CMAQ: A Decade in Review

Prakash Bhave, EPA/AMAD

- Tries to answer the question: "Has CMAQ performance for PM2.5 improved?"
- A: Yes, in general, by assessing in order:
  - Emissions
  - PBL height
  - Clouds
  - Wet removal
  - SOA chemistry

Conclusions





- Model performance has improved substantially!
- I've reviewed 8 major refinements to the modeling system.
  - →Meteorology inputs (2)
  - →Emissions & deposition (4)
  - →Atmospheric chemistry (2)

Updates to the Carbon Bond Mechanism for Version 6: CB6

Greg Yarwood and Jaegun Jung, ENVIRON; Gookyoung Heo, UT Austin; Gary Z. Whitten, SmogReyes; Jocelyn Mellberg, and Mark Estes, TCEQ

- CB last updated in 2005 (CB05)
- Update the core to 2010 state-of-science
- New aromatics chemistry (including toluene)
- New isoprene chemistry
- New ketone chemistry
- Explicit (non-lumping) of several species
- Optional Nitryl chloride (from sea salt) chemistry
- Optional Lightning NO_X

Summary of CB6 and CB05

	CB05	CB6	Change
Gas-phase reactions	156	218	+ 40%
Photolysis reactions	23	28	+ 22%
Gas-phase species	51	77	+ 50%
Emissions species for ozone	16	21	+ 31%

Some notable reaction rate changes from CB05 to CB6:

- $OH + NO_2 = HNO_3$ increased by 5% => greater radical sink
- $HCHO + h\nu = 2\ HO_2 + CO$ increased by 23% => greater radical source
- $NO_2 + h\nu = NO + O$ increased by 7% => more ozone
- $N_2O_5 + H_2O\ (+ H_2O) = 2\ HNO_3$ decreased by ~80%
    - Less NOx removal at night
    - Very important to include N_2O_5 reaction on aerosol surfaces

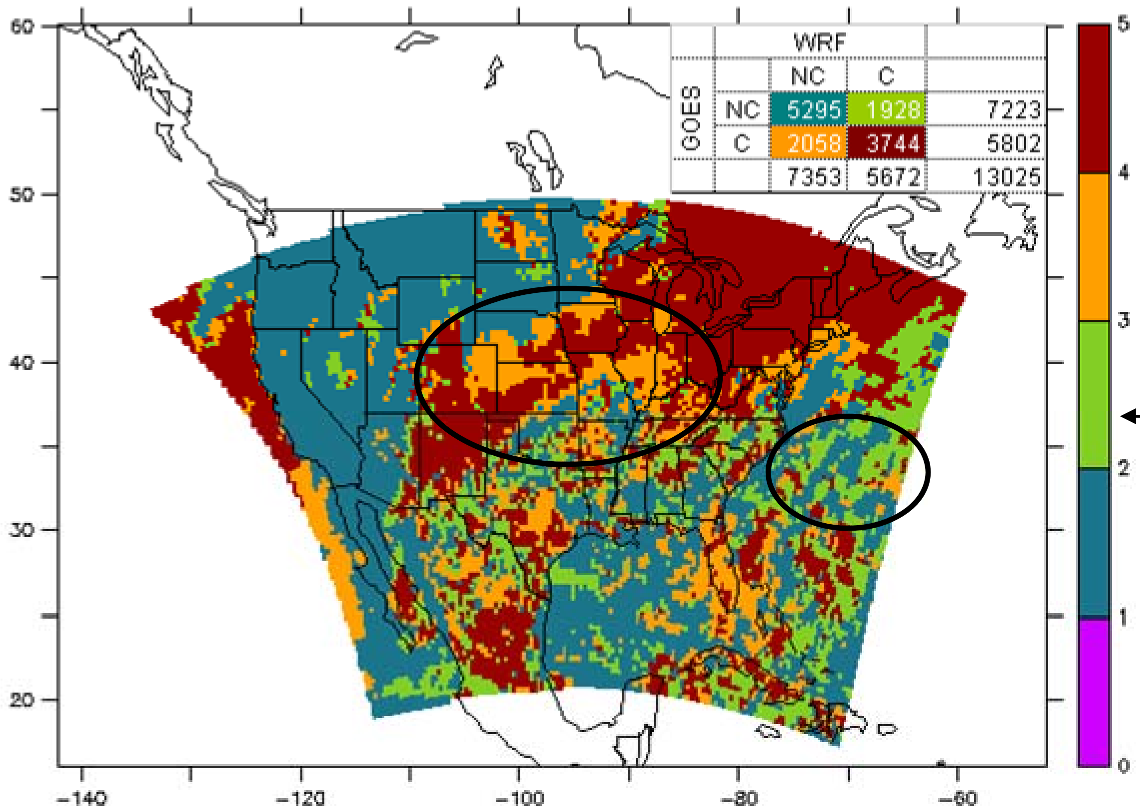
Use of Geostationary Satellite Observations for Dynamical Support of Model Cloud Fields

Arastoo Pour Biazar, Dick McNider, Kevin Doty, Yun-Hee Park, University of Alabama in Huntsville, Maudood Khan, The Universities Space Research Assoc., Bright Dornblaser, TCEQ

- The problem in cloud prediction is particularly frustrating in air quality SIP modeling since they are **retrospective simulations** in which the **observed cloud field is known from satellite observations** but models have significant differences in cloud placement.

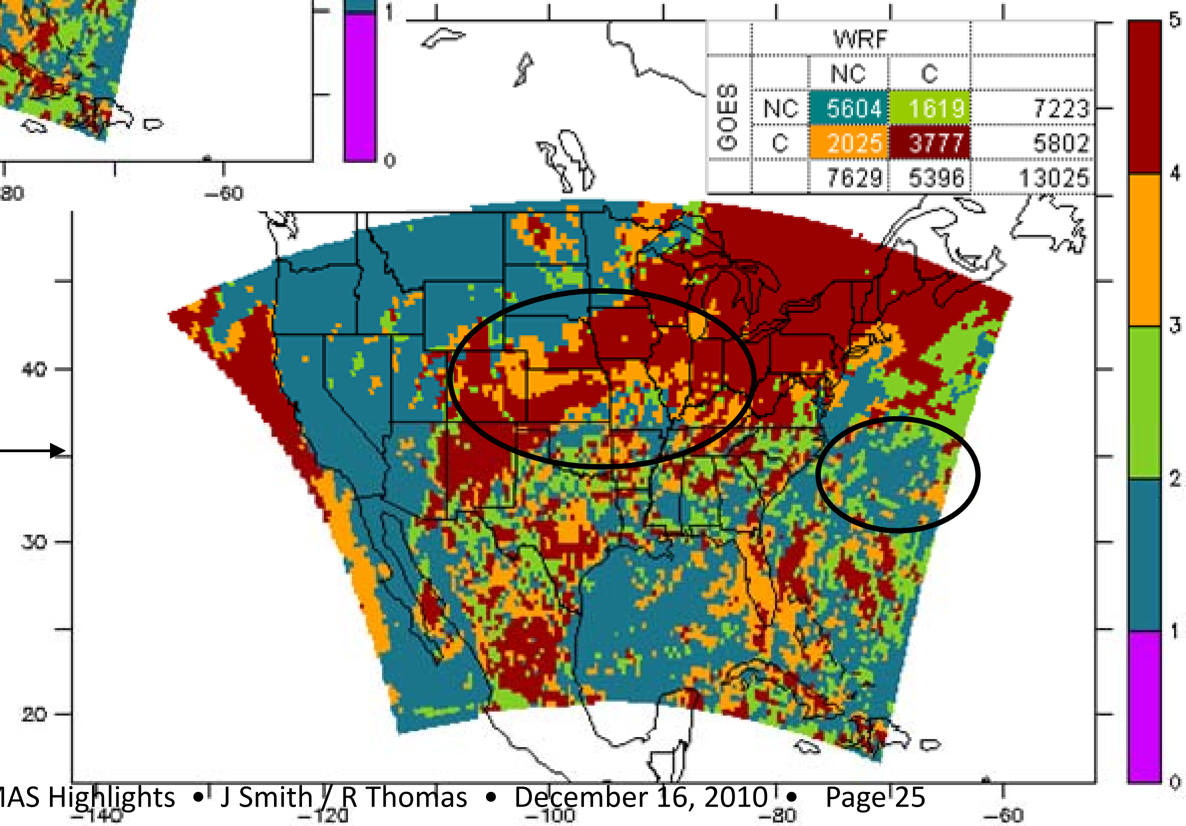
- The overall purpose of the current effort is **to improve model location and timing of clouds in the Weather Research and Forecast (WRF) meteorological model** which is widely used in the air quality planning community.

Preliminary Results



Control WRF simulation: August 19, 2006, 20 GMT

Satellite assimilation: August 19, 2006, 20 GMT



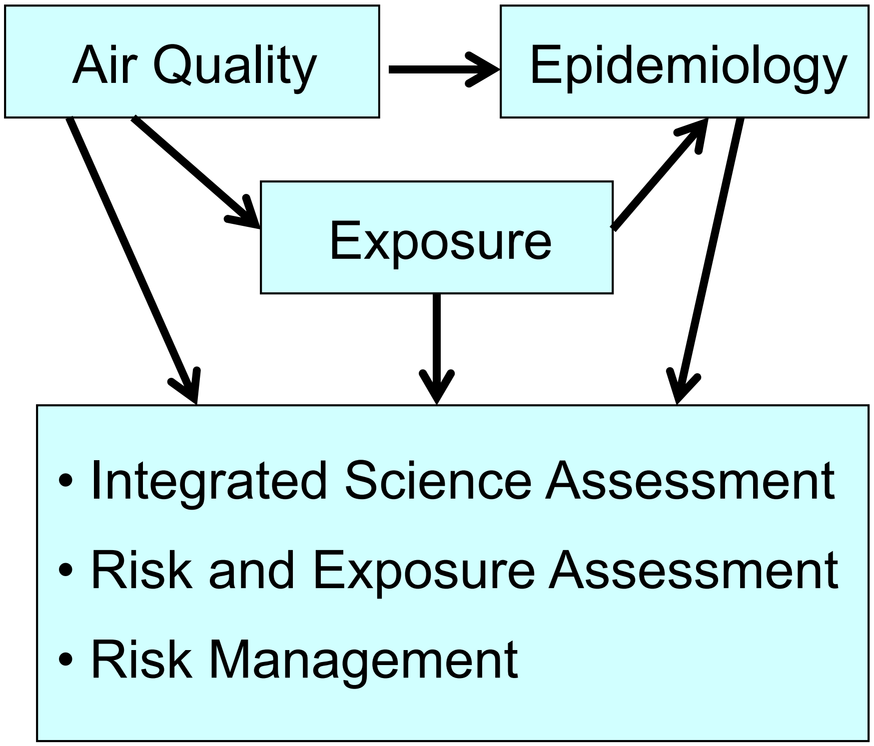
Air Pollution Health Studies:
Tying Air Quality to Epidemiology and Exposure

panels of experts and individual presentations

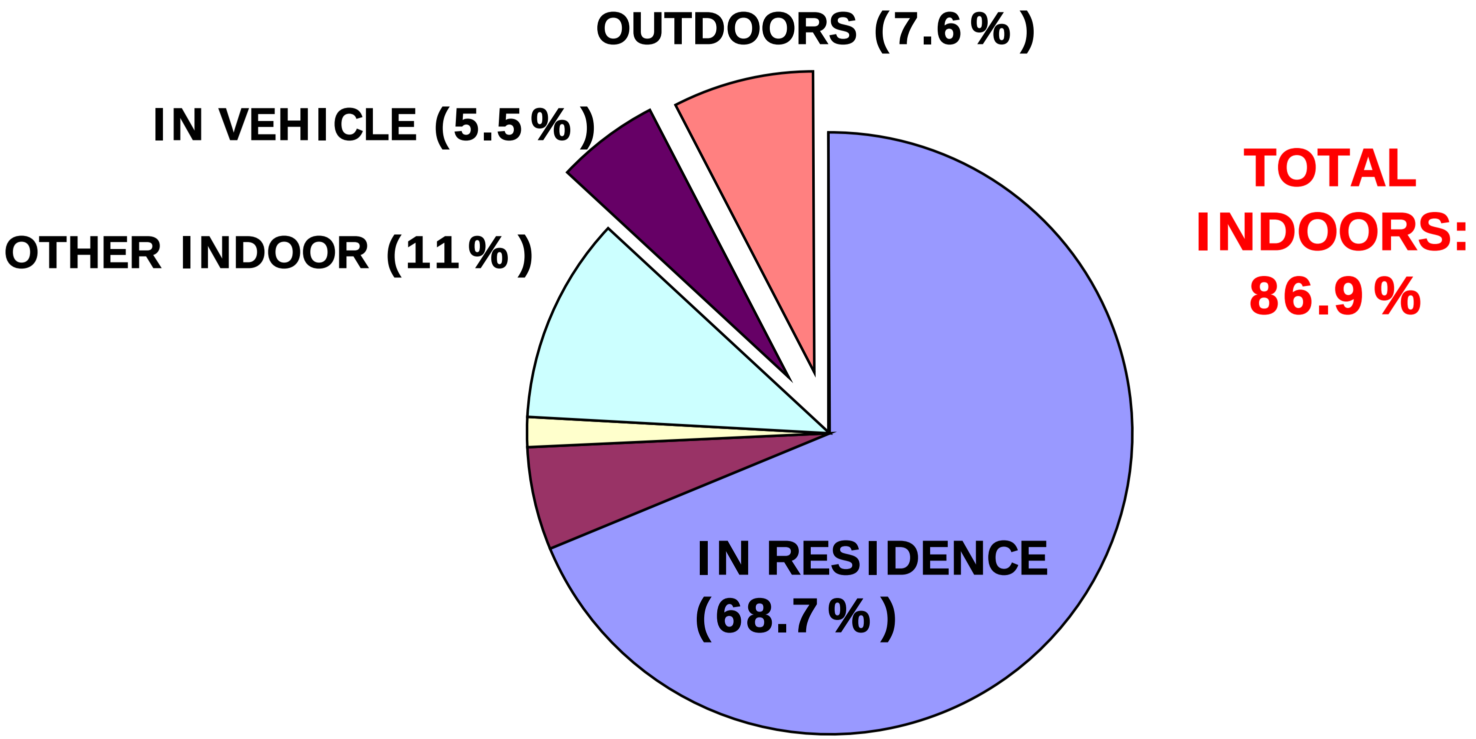
Role of Exposure Science and Epidemiology in Developing Air Quality Regulations and Controls

- Exposure science in risk assessment and risk management is critical to EPA's mission to promote public health and welfare
- EPA conducts exposure assessments to determine the route, magnitude, frequency, and distribution of exposure
- Epidemiology studies are vital in estimating the risk and the impact of air pollution on human health.
- Latest research in epidemiology emphasizes the need for more reliable estimates or surrogates of human exposures

Role of Exposure Science and Epidemiology in EPA



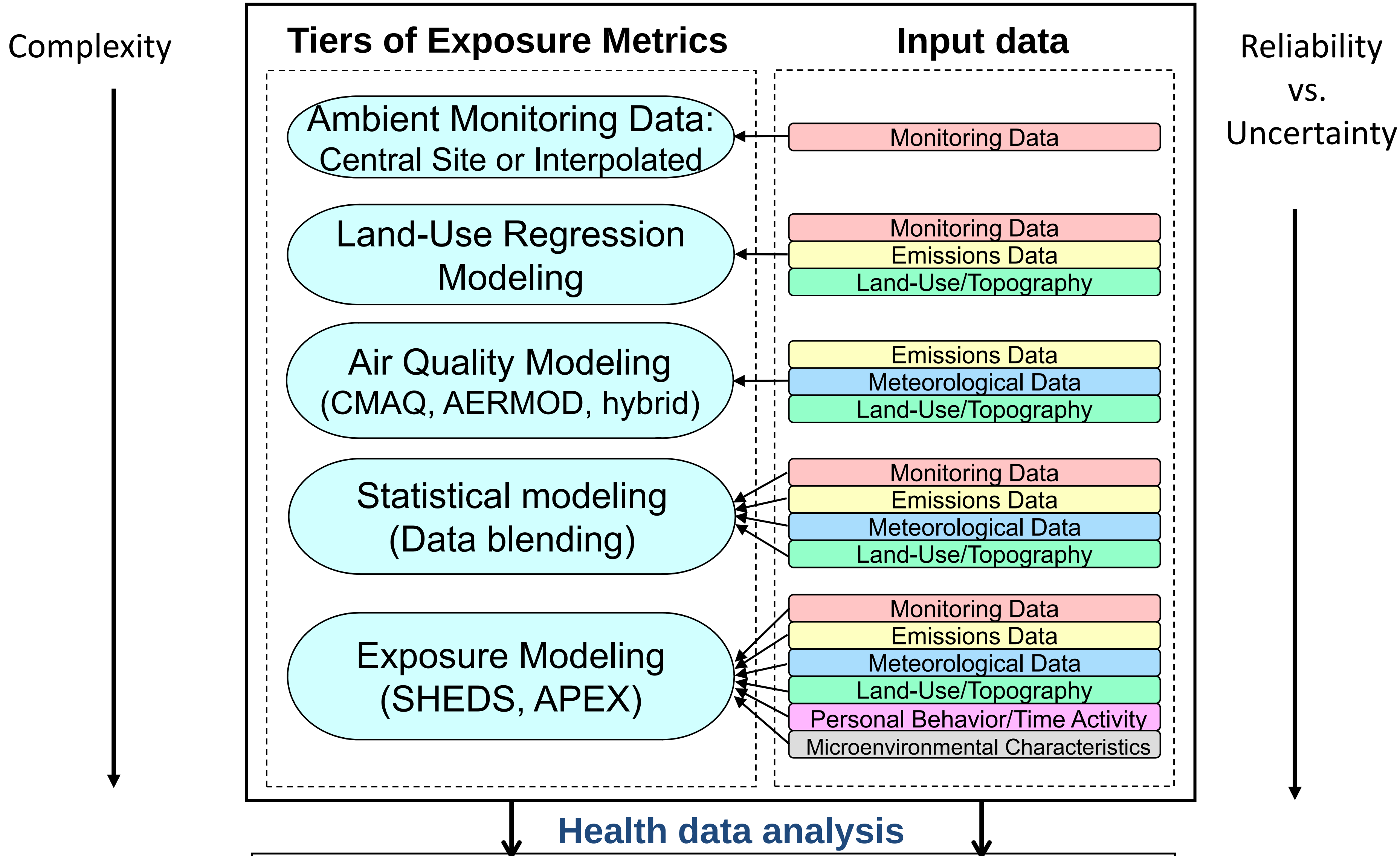
Average Time Spent in Each Microenvironment



National Human Activity Pattern Survey (NHAPS)

Adapted by Klepeis et al., 2001

Exposure Information Relevant to Health Studies



Epidemiological statistical models:

$\log(E(Y_{kt})) = \alpha + \beta\ \textit{exposure metric}_{kt} + \sum_k \gamma_k \textit{area}_{kt} + \ldots \textit{other covariates}$

Stochastic Human Exposure and Dose Simulation (SHEDS) Model for Air Pollutants