Work Plan for the Development, Application, and Evaluation of Global-Through-Urban WRF/Chem to Study the Impact of Global Change on Air Quality

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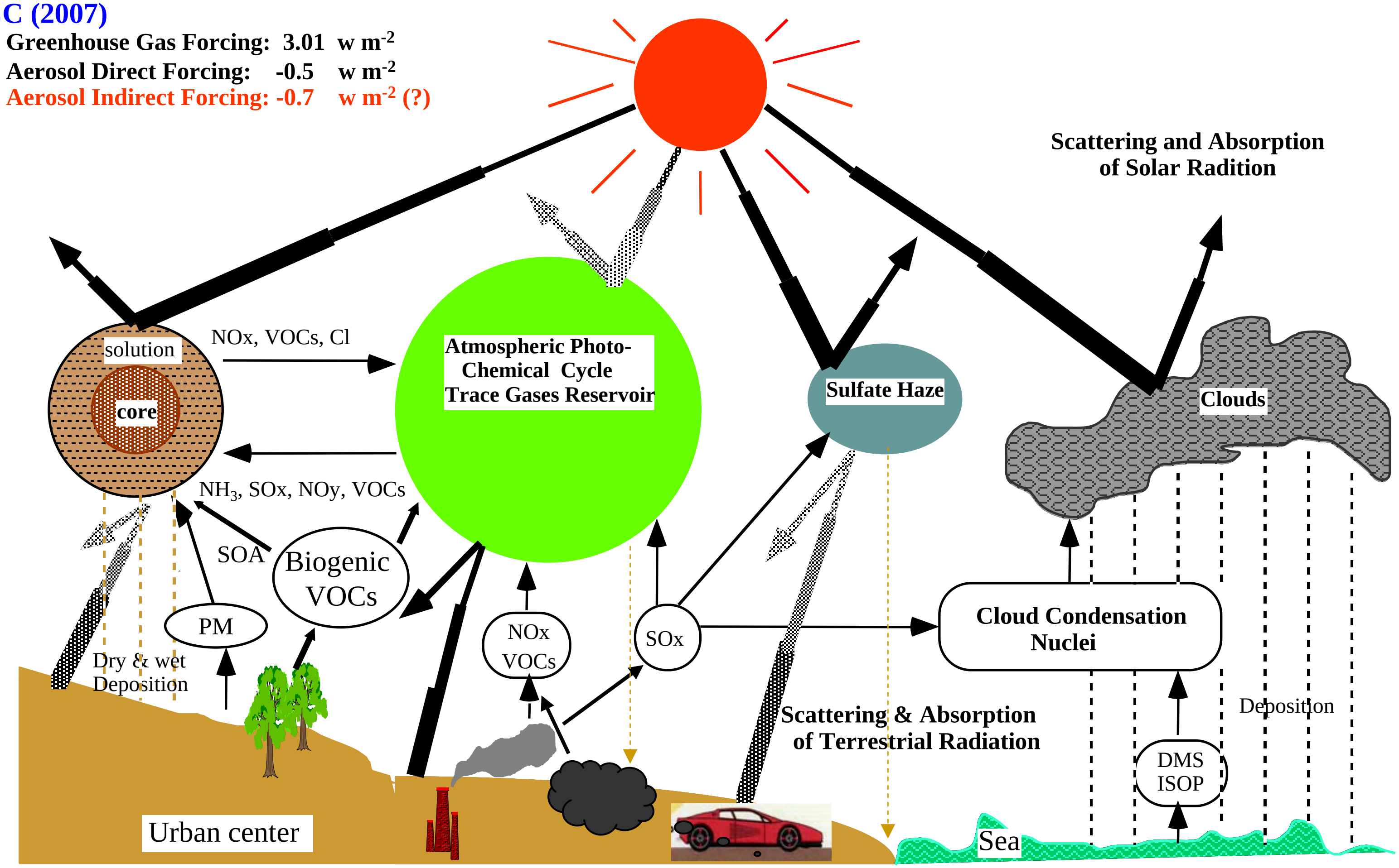
One Atmosphere

Aerosols, Gases, Chemistry, Transport, Climate

IPCC (2007)

Greenhouse Gas Forcing: 3.01 w m^{-2}
Aerosol Direct Forcing: -0.5 w m^{-2}
Aerosol Indirect Forcing: -0.7 w m^{-2} (?)



Coupling Air Quality/Climate Modeling:
History and Current Status

- **Prior to 1994: Separation of Air Quality/Climate**
- **1994-Present: Coupling of Air Quality/Climate**
  - **Urban/Regional Models**
    - **The first fully-coupled meteorology/chemistry/aerosol/radiation model, GATOR-MMTD, was developed by Jacobson in 1994**
    - **The first community coupled meteorology/chemistry/aerosol/radiation model, WRF/Chem, was developed by Grell et al. in 2002**
    - **Most air quality models (AQMs) are still offline**
    - **Most AQMs do not treat aerosol direct and indirect effects**
    - **Most regional climate models use prescribed aerosols or simple modules without detailed aerosol microphysics**
  - **Global Models**
    - **The first nested global-through-urban scale fully-coupled model, GATOR-GCMM, was developed by Jacobson in 2001**
    - **Most global AQMs (GAQMs) are still offline**
    - **Most GAQMs use an empirical sulfate-CCN relation for indirect effects**

Background and Motivation

- Common deficiencies of a global climate-aerosol model
  - Coarse spatial resolution cannot explicitly capture the fine-scale structure that characterizes climatic changes (e.g., clouds, precipitation, mesoscale circulation, sub-grid convective system, etc.) and air quality responses
  - Coarse time resolution cannot replicate variations at smaller scales (e.g., hourly, daily, diurnal)
  - Simplified treatments (e.g., simple met. schemes and chem./aero. treatments) cannot represent intricate relationships among meteorology/climate/AQ variables
  - Most models simulate climate and aerosols offline with inconsistencies in transport and no climate-chemistry-aerosol-cloud-radiation feedbacks
- Common deficiencies of a urban/regional climate or AQ model
  - Most AQMs do not treat aerosol direct and indirect effects
  - Most AQMs use offline met. fields without feedbacks
  - Some AQMs are driven by a global model with inconsistent model physics
  - Most regional climate models use prescribed aerosols or simple modules without detailed chemistry and aerosol microphysics

Hypotheses, Scientific Questions, and Objectives

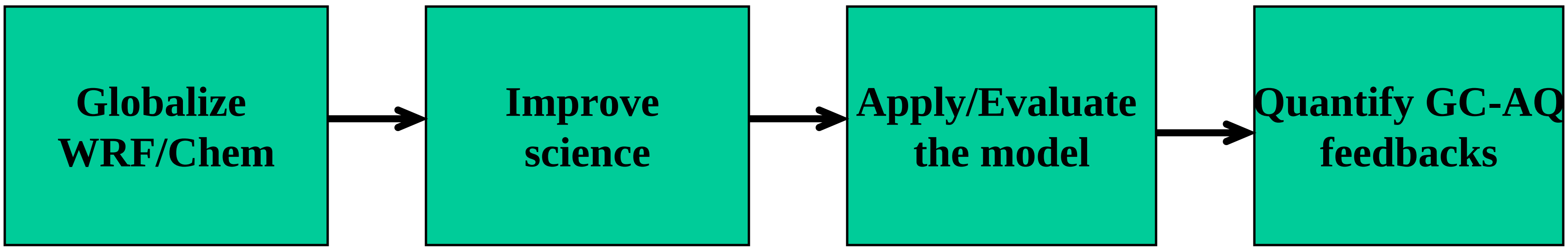
- **Hypothesis**
  - **Two-way feedbacks between climate changes and air quality (AQ) are important in quantifying the impact of global changes (GC) on AQ**
- **Scientific Questions**
  - **What are the potential effects of GC on the abundance and properties of trace gases and aerosols on urban/regional scales?**
  - **How important are the two-way GC and AQ feedbacks? What is the relative importance of aerosol direct and indirect effects?**
  - **What are the key uncertainties associated with the predicted effects?**
- **Objectives**
  - **Develop a global-through-urban (GU) WRF/Chem**
  - **Conduct 2-way nesting simulations for current/future scenarios**
  - **Examine the sensitivity of model predictions to model parameters**
  - **Quantify the effects of GC on AQ via direct and indirect feedbacks**

Weather Research and Forecast/Chemistry Model (WRF/Chem): An Overview

- History
  - First version developed by NOAA/FSL and released in 2002
- Main Developers and Collaborators
  - NCAR/MMM, NOAA/ESRL, PNNL, NCSU, BAMS, and others
- Main Features
  - Online coupling of meteorology and chemistry to allow climate-aerosol-chemistry-cloud-radiation feedbacks
  - 1- or 2-way nesting on scales from freeway to continental, potentially global
  - All transport done by the meteorological model to ensure consistency
  - Aerosol direct and indirect radiative forcing
  - Modularity to facilitate model development and module inter-comparison
  - Community model for research and operational applications
  - Four gas-phase chemical mechanisms
    - RADM2, RACM, CBMZ, and CB05
  - Three aerosol modules
    - MADE/SORGAM, MOSAIC, and MADRID

Overall Approach and Challenges

- **Overall Approach**



- **Key Challenges**
  - **Projection from conformal to non-conformal (Caltech/NCAR)**
  - **Development of an adequate global emission inventory**
  - **Develop appropriate model treatments for chemistry and aerosol/cloud microphysics for troposphere & stratosphere**
  - **Nesting between global and regional domains with mass conservation and consistency**
  - **Computational efficiency and accuracy trade off**

Technical Approaches and Tasks: Emissions (ANL + NCSU)

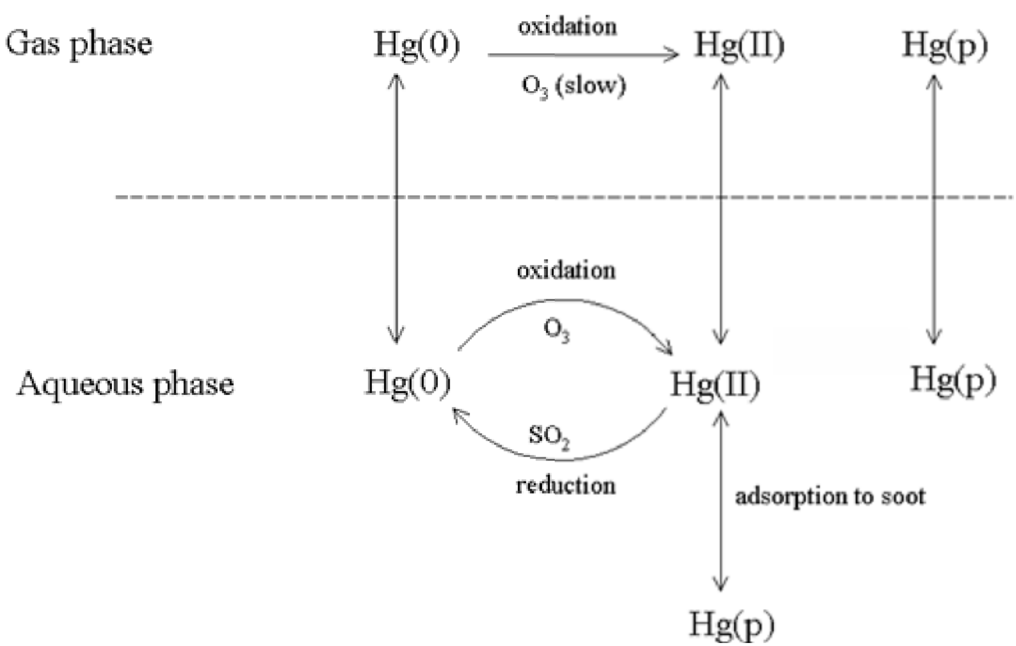
- **Current (2001)**
  - **Species: SO_2, NO_x, NMVOCs, CO, CO_2, CH_4, N_2O, NH_3, CFCs, HCFCs, Hg(0), Hg(II) (gas+PM), PM (sulfate, BC, POM, dust, sea-salt)**
  - **Global: IPCC-SRES, GEIA, GMEI, AeroCom**
  - **Regional: NEI99 (or 05), AMEI, CMU-NH_3, ANL-Asian emissions, AER-Hg, updated ANL East Asia inventory**
- **Future (2010, 2020, 2030, 2040, 2050)**
  - **Growth factors by regions, species, emitting factor, and energy changes**
  - **Four IPCC scenarios: A1B, A2, B1, and B2 (or equivalent in IPCC 2007)**
- **Online meteorology-dependent emission modules**
  - **Biogenic species**
  - **Sea-salt**
  - **Wind-blown dust**

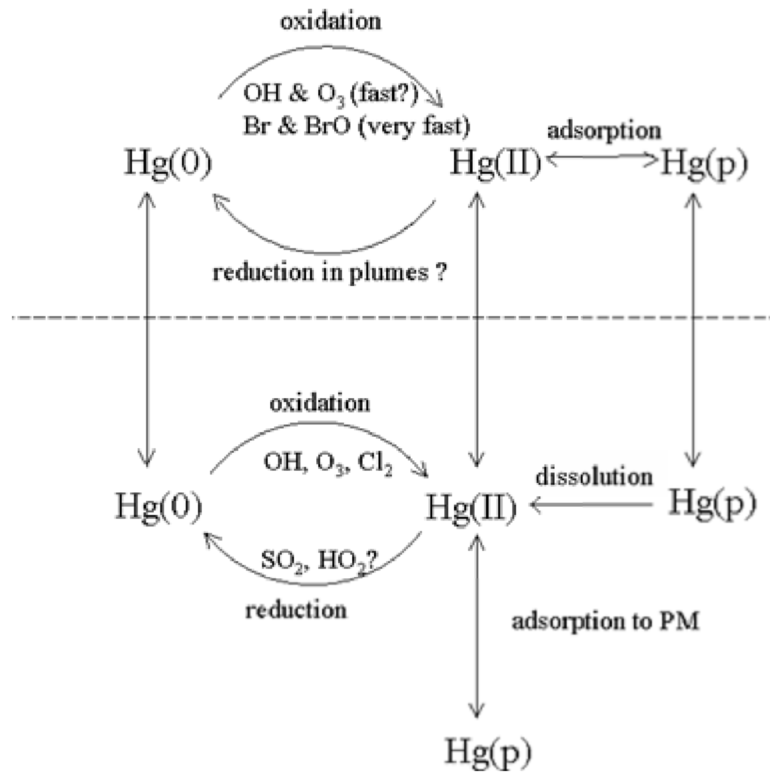
Technical Approaches and Tasks:

GU-WRF/Chem Model Development (NCSU + AER)

- **Extension of CB05 for Regional and Global Atmospheres**
  - **EPA CB05+tropospheric Cl chemistry**
  - **Additional oxidant reactions for low stratosphere (< 30 km)**
  - **Additional halogen reactions needed for stratospheric and Hg-chemistry**
- **Addition of Mercury Chemistry into CB05**
  - **EPA and AER Hg-mechanisms with new science**
    - **Gas: oxidation of Hg(0) to Hg(II) (e.g., O_3, H_2O_2, OH, Br, and BrO)**
    - **Aqueous: oxidation of Hg(0) to Hg(II) and reduction of Hg(II) to Hg(0)**
    - **PM: adsorption/desorption of Hg(II)**
- **Incorporation of Plume-in-Grid Treatments**
  - **AER's APT with consistent chemistry and PM treatments with WRF/Chem**
  - **Development of interface, pre- and post-processors**
- **Development/Improvement of PM Treatments**
  - **Update MADE/SORGAM in WRF/Chem based on CMAQ**
  - **Incorporate new science into SOA module (e.g., isoprene SOA)**
  - **Implement a new aerosol activation parameterization**

Evolution of Model Treatments of Mercury Chemistry
1994 vs. 2007 (Lindberg et al., 2007)



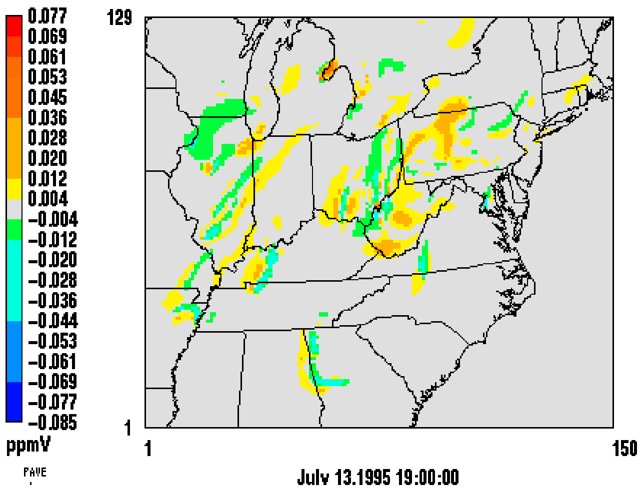


12 years ago
(Source: Mercury Expert Panel, 1994)

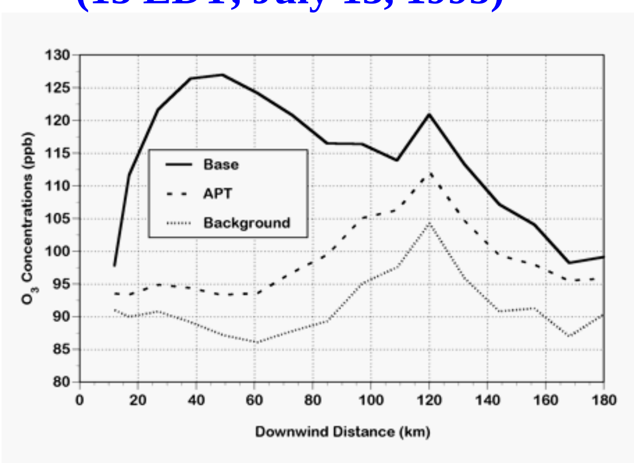
Present-day

Effects of Plume-In-Grid Treatments
(Karamchandani et al., 2002; 2006)

Surface O_3 (APT-Base)

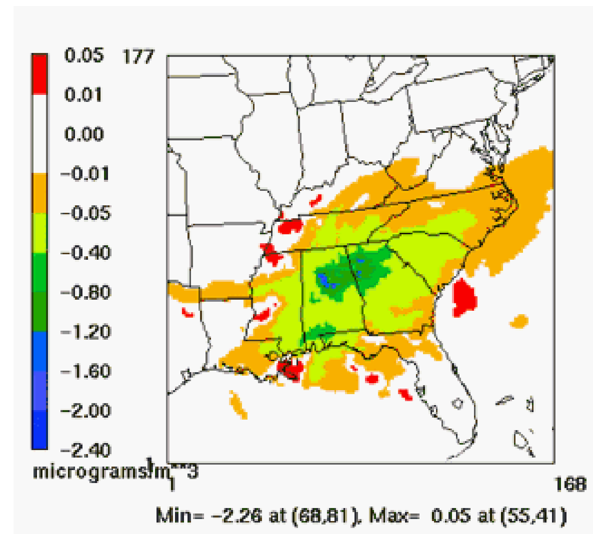


Surface O_3 downwind of NC Point Source (15 EDT, July 13, 1995)

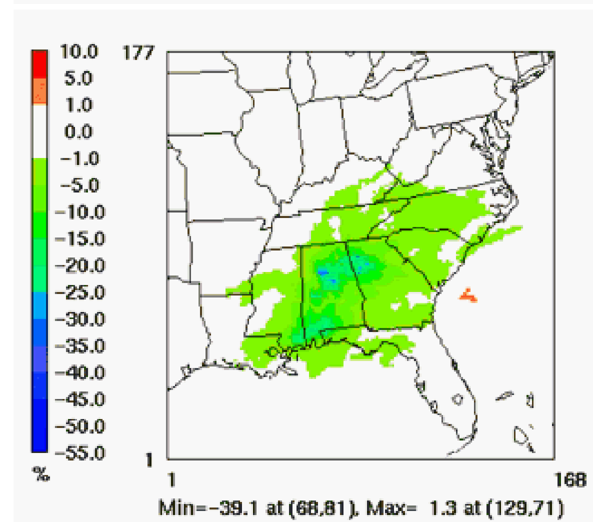


$PM_{2.5}$ Sulfate

Absolute Difference (APT-Base)

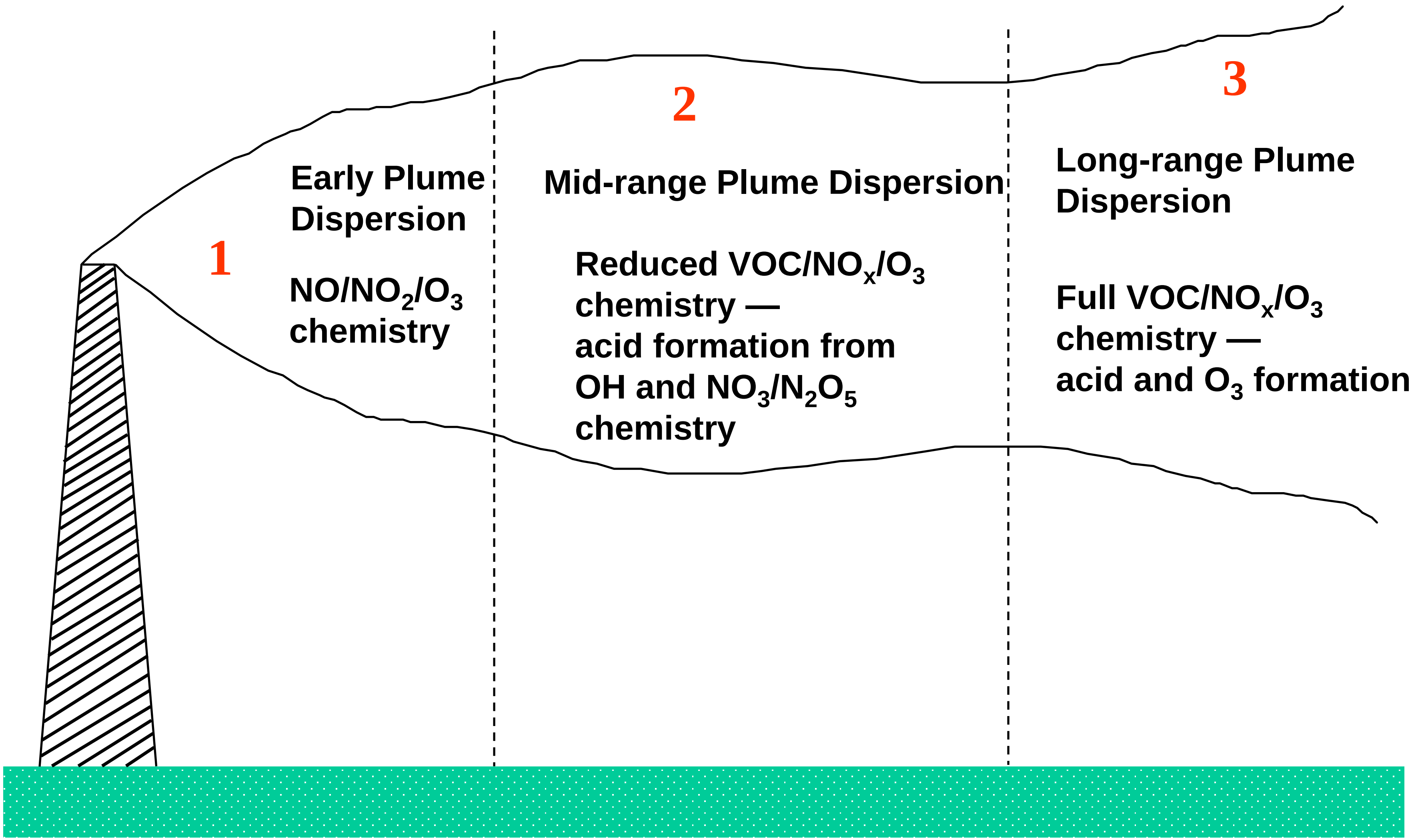


Percent Difference



Plume Chemistry & Relevance to PM Modeling

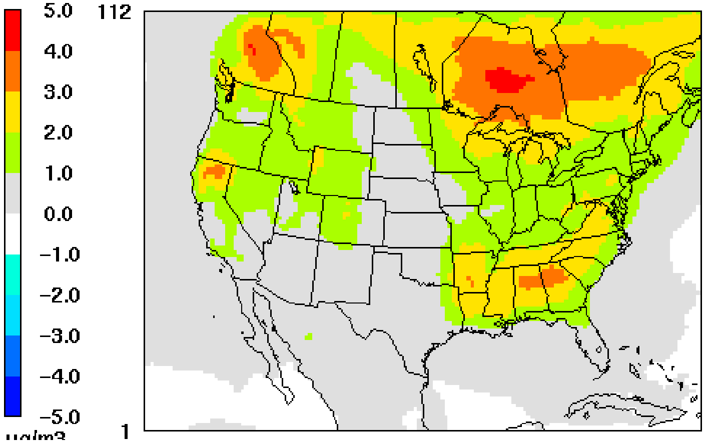
(Karamchandani et al., 2005, 2006)



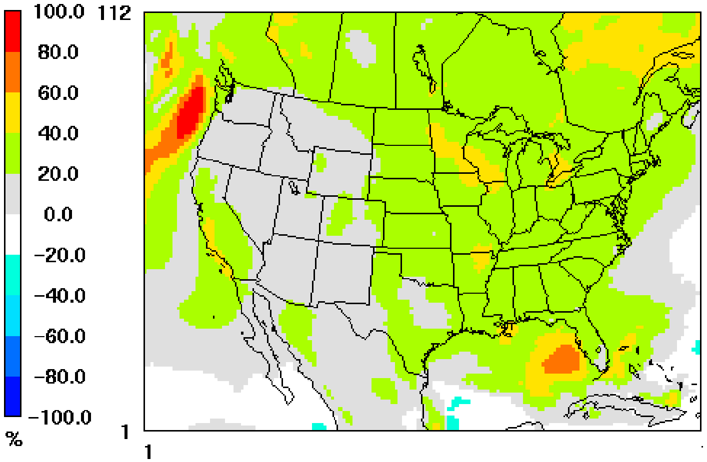
Contributions of Isoprene to Biogenic SOA in 2001

Summer (JJA)

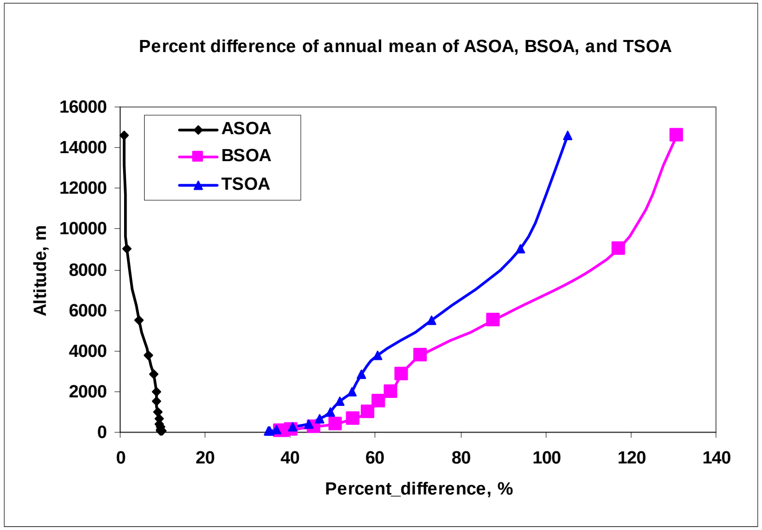
Absolute difference



Percent difference



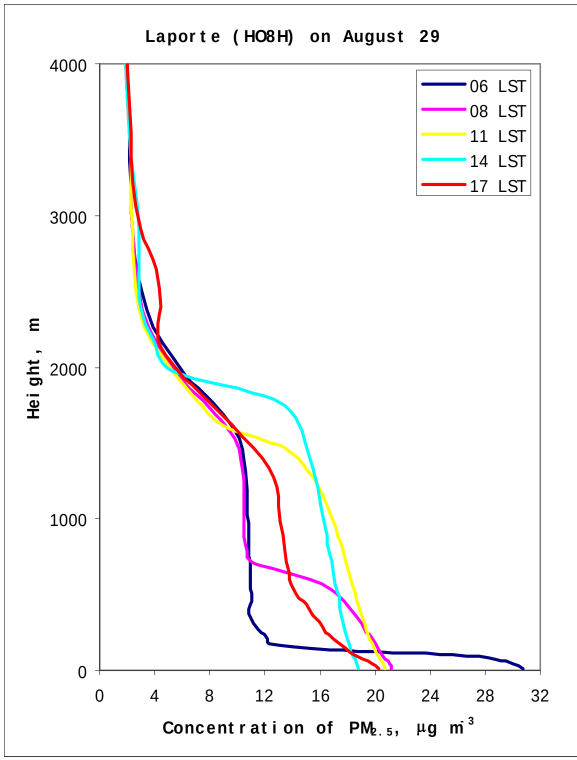
Annual

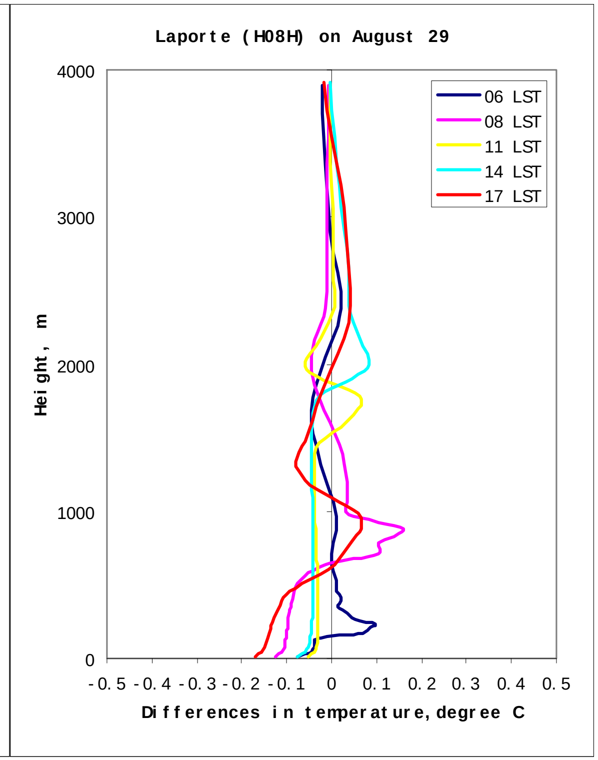


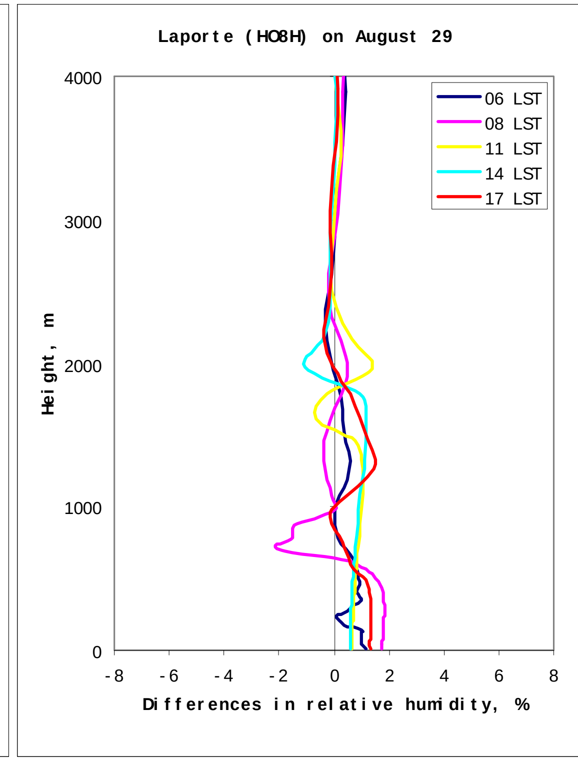
BSOA increases by < 4.3 μg m^{-3} (up to 107%) in PBL (0-2.9 km)

Feedbacks of Aerosols to T and RH (LaPorte, TX)

$PM_{2.5}$ **(Gas+PM - Gas only)**





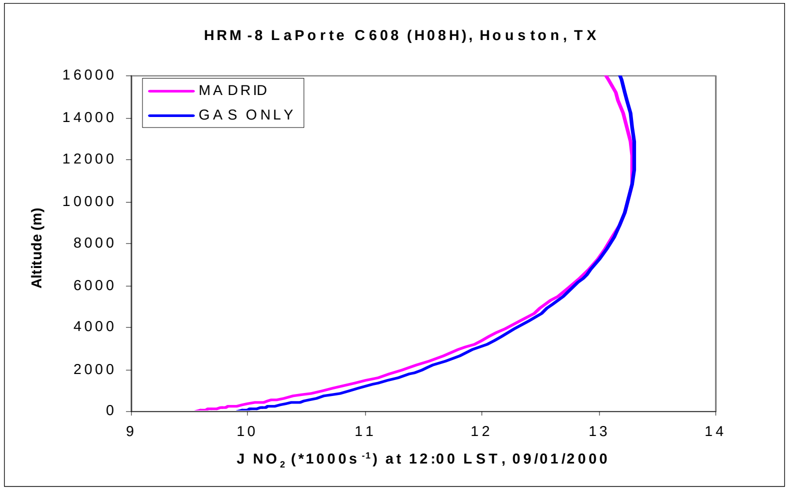


Diff > 0, T(RH) increases (decreases) due to aerosol feedbacks

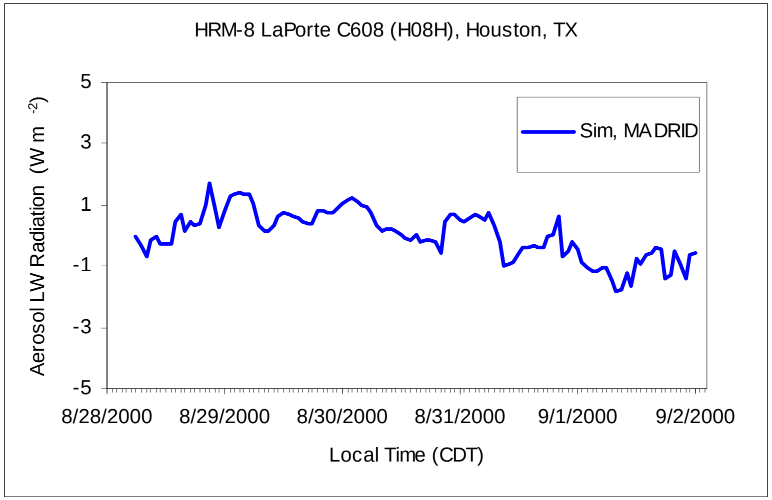
Diff < 0, T(RH) decreases (increases) due to aerosol feedbacks

Feedbacks of Aerosols to NO_2 Photolysis and Radiative Forcing

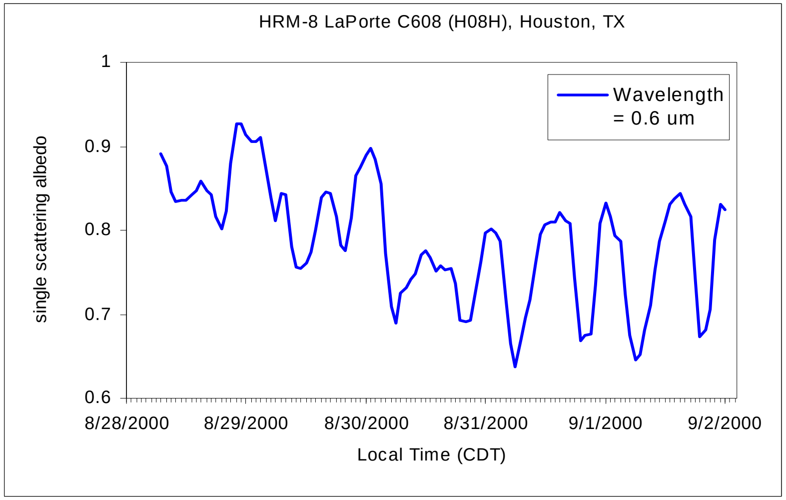
NO_2 Photolysis



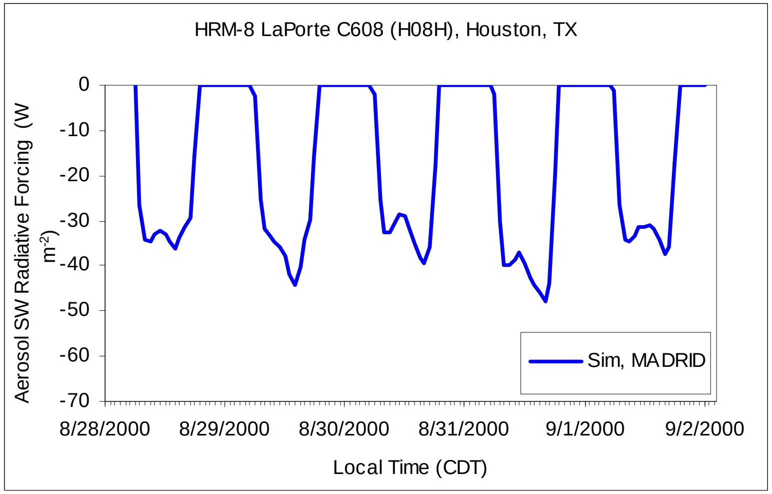
LW Radiative Forcing



Single Scattering Albedo

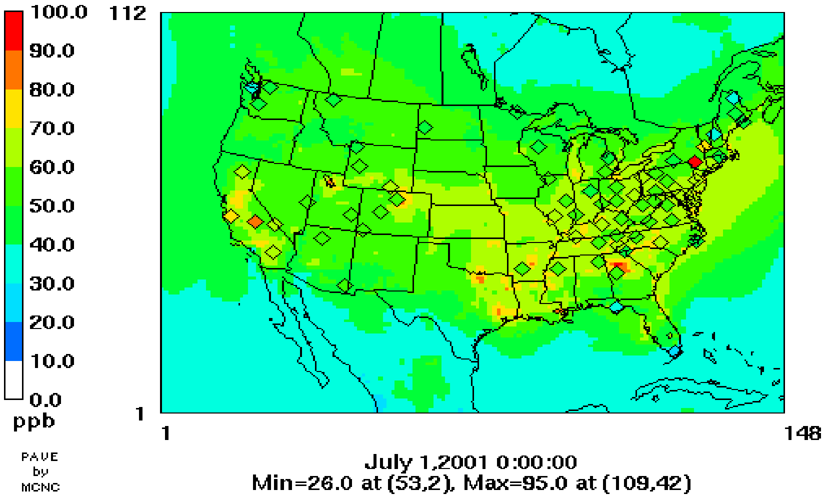


SW Radiative Forcing

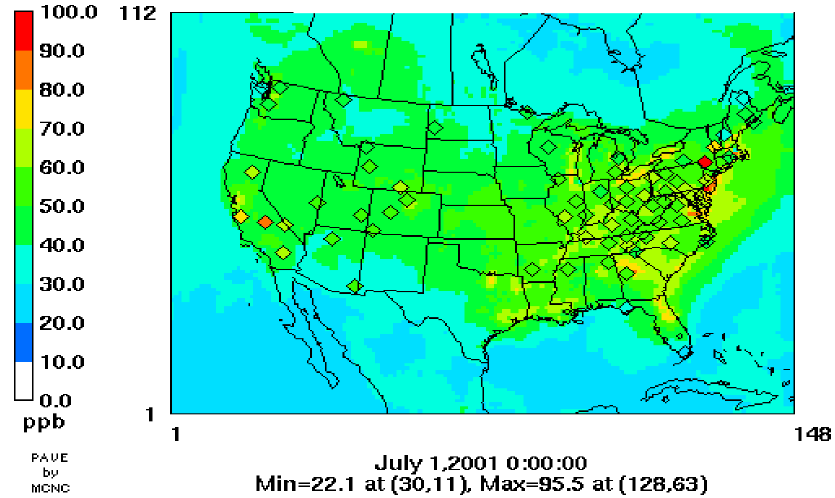


Weekly Mean Max 1-hr Average O_3 (CASTNet)

MM5/CMAQ-CB05

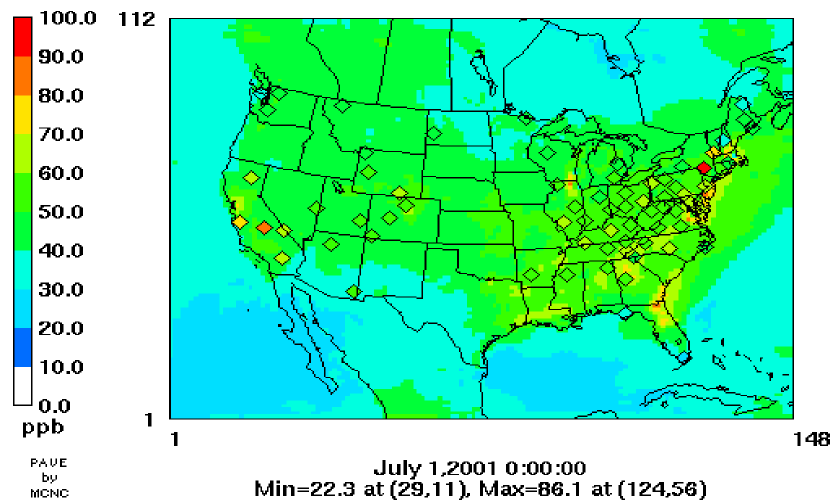


WRF/Chem-CB05

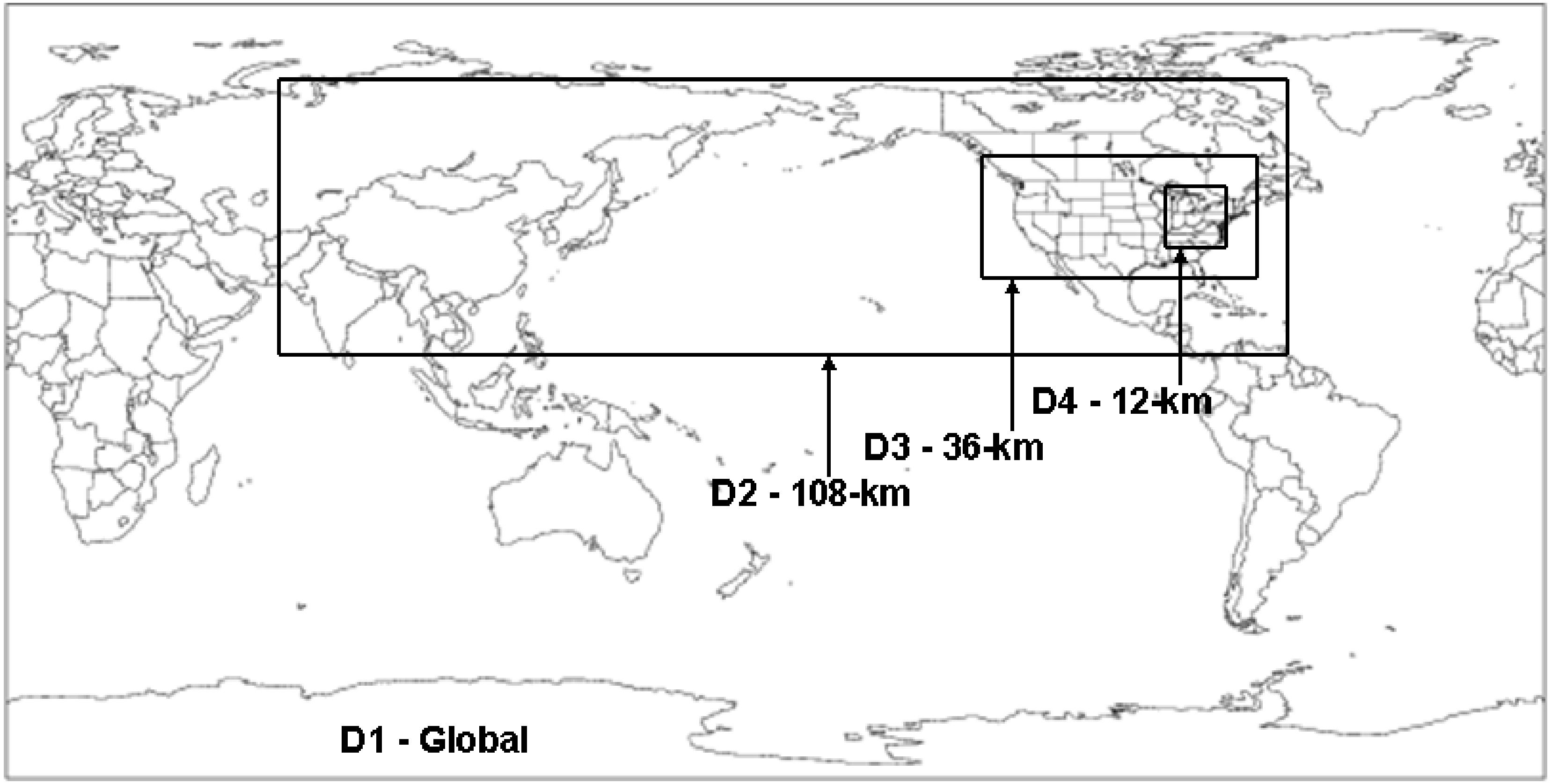


	Cr	RMSE	NMB
MM5/CMAQ-CB05	0.59	11.5	13%
WRF/Chem-CB05	0.32	17.0	9%
WRF/Chem-CBMZ	0.35	16.2	8%

WRF/Chem-CBMZ



Technical Approaches and Tasks:
Modeling Domains



Technical Approaches and Tasks:
Model Application (NCSU)

- **Current:**
  - **WRF vs. WRF/Chem, 2001, D1, D2, D3**
- **Future:**
  - **WRF/Chem, IPCC A1B/B2, 2050, D1, D2, D3**
  - **WRF/Chem, IPCC A1B, decadal increment for summer/winter**
- **Sensitivity:**
  - **Model inputs (e.g., Asian emissions)**
  - **Model configurations (e.g., 1- vs. 2-way nesting, coarse vs. fine grid)**
  - **Model formulations (e.g., w. and w/o PinG, w. and w/o aerosol indirect forcing, MADE/SORGAM vs. MADRID)**

Technical Approaches and Tasks:
Model Evaluation and Analyses (NCSU)

- **Datasets and Model Intercomparison**
  - **Current**
    - **AeroCOM: MODIS, POLDER, MISR, AVHHR, SEAWIFS, TOMS, AERONET and surface data**
    - **Surface/vertical: CASTNet, IMPROVE, AIRS/AQS, STN, NADP, AIRMon, MDN, SEARCH, CRPAQS, NWS, NCEP**
    - **Satellite: MOPITT, POAM III, GOMOS, MIPAS,**
  - **Future**
    - **WRF vs. MM5 (Mickley et al., 2004; Lueng et al., 2003, 2005)**
- **Evaluation/Analysis Protocol**
  - **Operational, diagnostic, and mechanistic**
  - **Temporal, spatial, and statistical**
  - **Meteorological and chemical predictions**

Expected Results

- **A global-through-urban WRF/Chem that contains the state-of-the science treatments for gases, PM, and Hg**
- **A revised CB05 that is suitable for urban-to-global applications in both troposphere and stratosphere**
- **A realistic assessment of the effects of global changes on air quality with 2-way nesting from a unified model**
- **An improved understanding of the associated sensitivities /uncertainties by accounting for 2-way feedbacks**
- **Several peer-reviewed publications**

Acknowledgments

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- **Naresh Kumar and Eladio Knipping, EPRI and Christian Seigneur, AER, for providing MADRID and APT codes**
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- **Mark Estes, TCEQ, for providing 2001 observational data collected by TCEQ**
- **Carey Jang and Sharon Phillips, U.S. EPA, for helpful discussions on coupled meteorology and air quality models**

Tasks and Timelines

	Months from the Project Start					
Tasks	6	12	18	24	30	36
1. Preparation of Emission Inventories						
1a Emissions for Present-Year Scenarios	■		■			
1b Emissions for Future-Year Scenarios		■	■	■	■	
1c Implementation of Online Emission Modules	■	■				
2. Model Development and Improvement						
2a Extension of CB05 for Regional and Global Atmospheres	■					
2b Addition of Mercury Chemistry into CB05	■	■				
2c Development/Improvement of PM Treatments	■	■				
2d Incorporation of Plume-in-Grid Treatments		■	■			
3. Model Simulations						
3a Current-Year Simulation (C1-C2)		■	■			
3b Future-Year Simulations (F1-F6)			■	■	■	
3c Sensitivity Simulations (S1-S5)				■	■	■
4. Model Evaluation						
4a Obtain/Prepare Datasets for Model Evaluation	■	■				
4b Evaluate/Interpret Current-Year Simulation			■	■	■	
4c Evaluate/Interpret Future-Year/Sensitivity Simulations				■	■	■