

US EPA ARCHIVE DOCUMENT

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

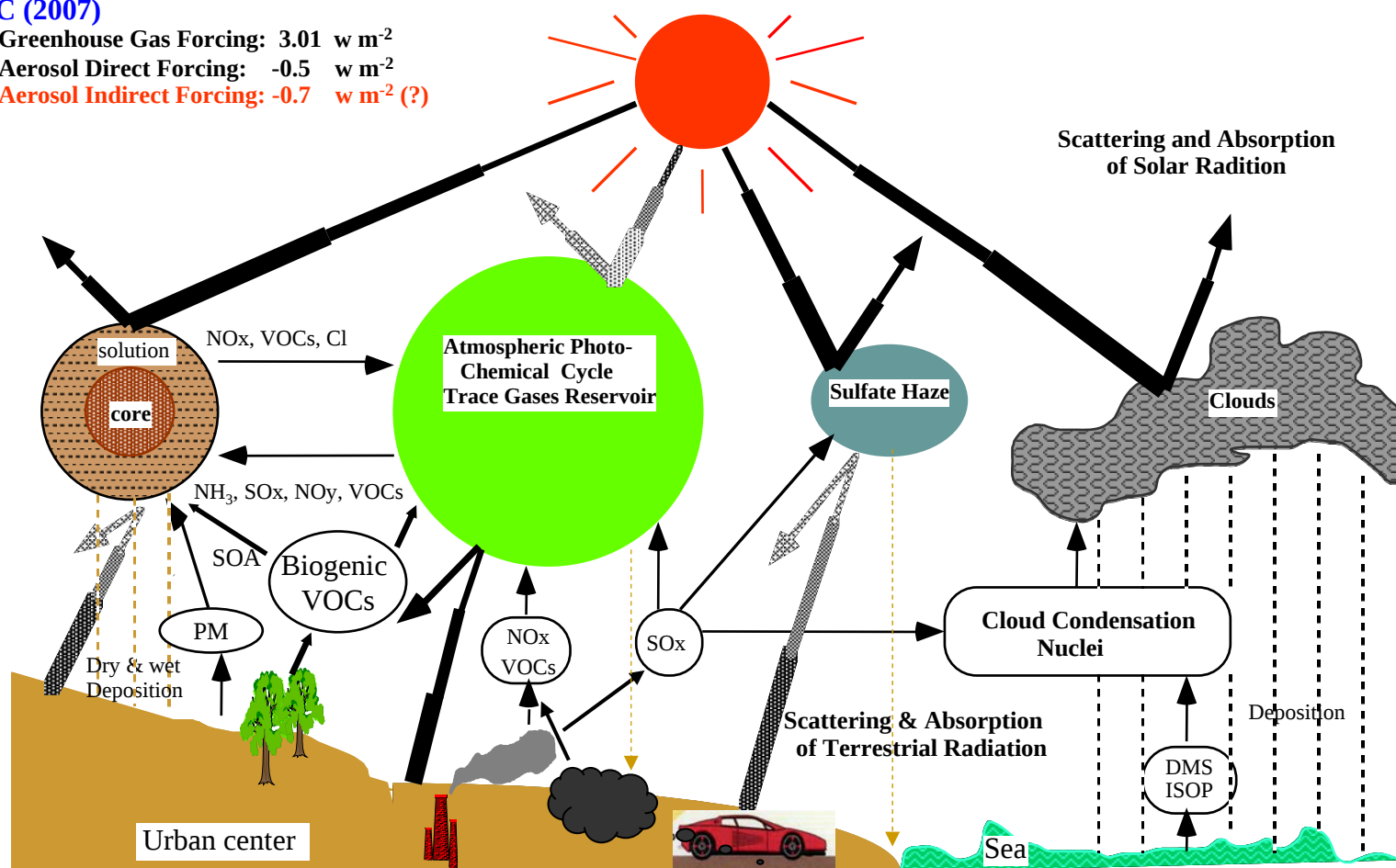
Aerosols, Gases, Chemistry, Transport, Climate

IPCC (2007)

Greenhouse Gas Forcing: 3.01 W m^{-2}

Aerosol Direct Forcing: -0.5 W m^{-2}

Aerosol Indirect Forcing: $-0.7 \text{ W m}^{-2} (?)$



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**

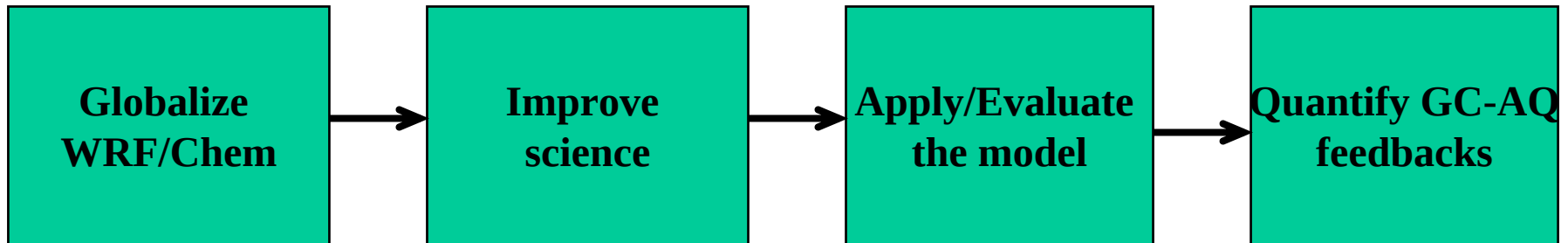
- Develop a global-through-urban (GU) WRF/Chem
- Conduct 2-way nesting simulations for current/future scenarios
- Examine the sensitivity of model predictions to model parameters
- Quantify the effects of GC on AQ via direct and indirect feedbacks

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: SO₂, NO_x, NMVOCs, CO, CO₂, CH₄, N₂O, NH₃, 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-NH₃, 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

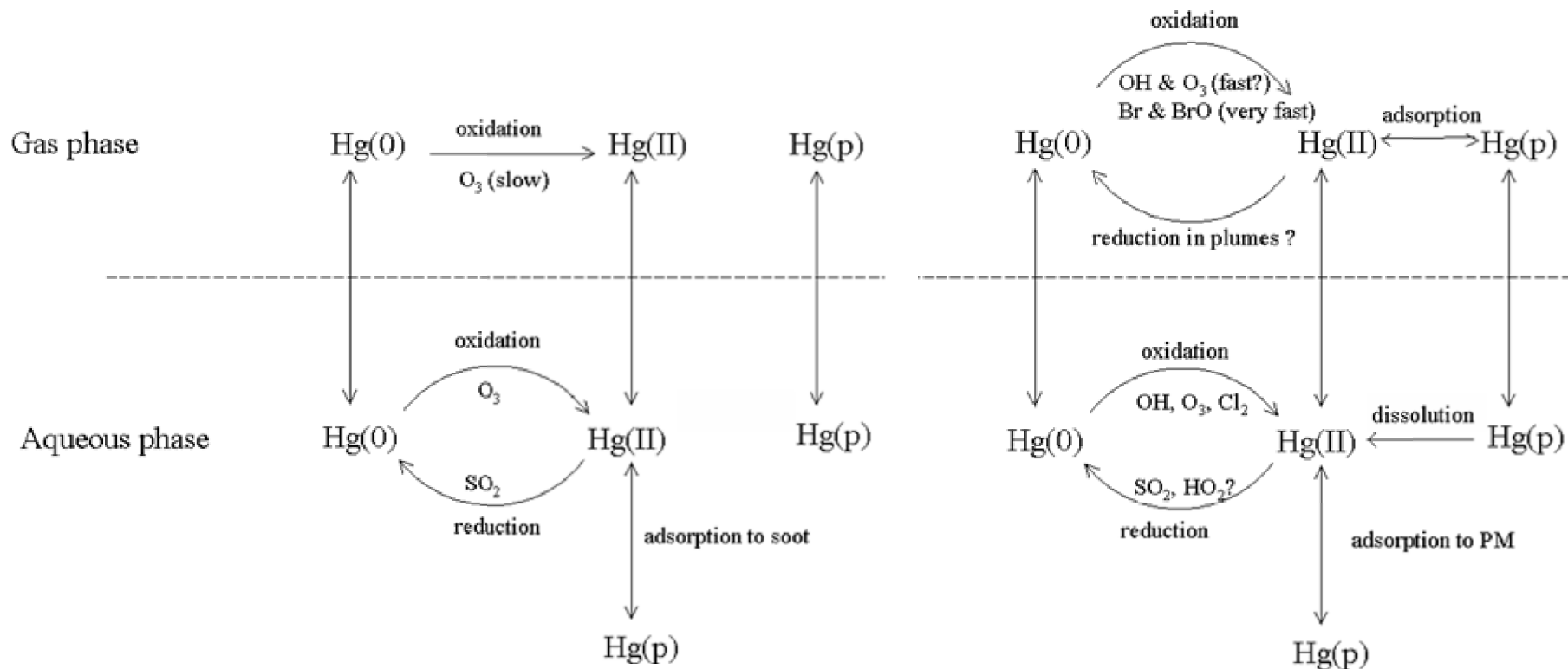
Technical Approaches and Tasks:

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., O₃, H₂O₂, 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

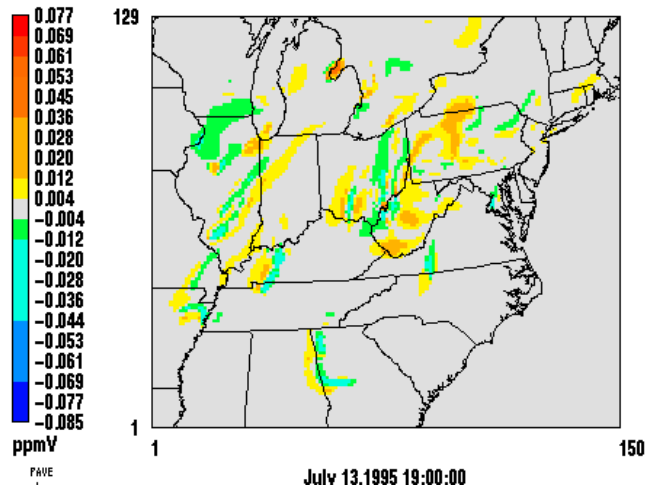
(Source: Mercury Expert Panel, 1994)

Present-day

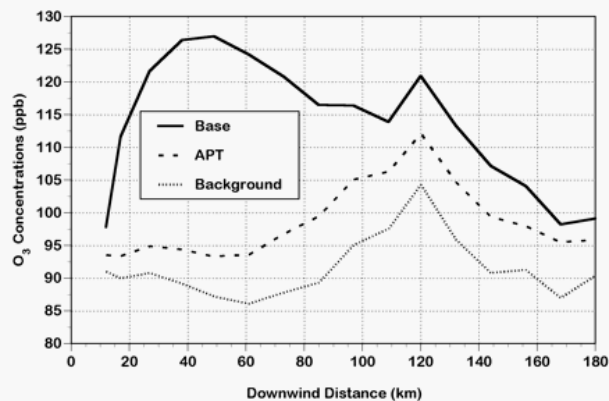
Effects of Plume-In-Grid Treatments

(Karamchandani et al., 2002; 2006)

Surface O₃ (APT-Base)

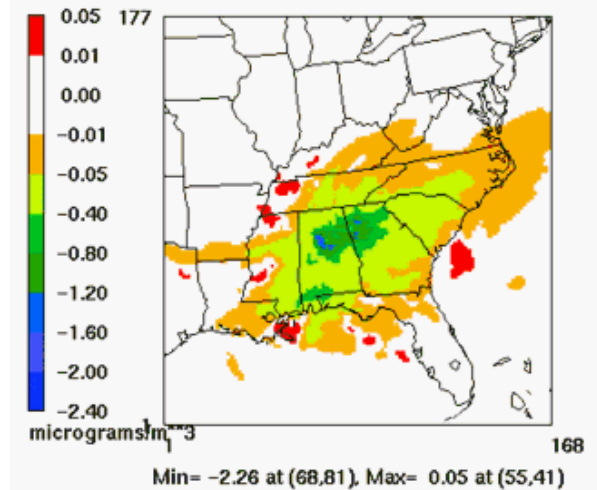


Surface O₃ downwind of NC Point Source
(15 EDT, July 13, 1995)

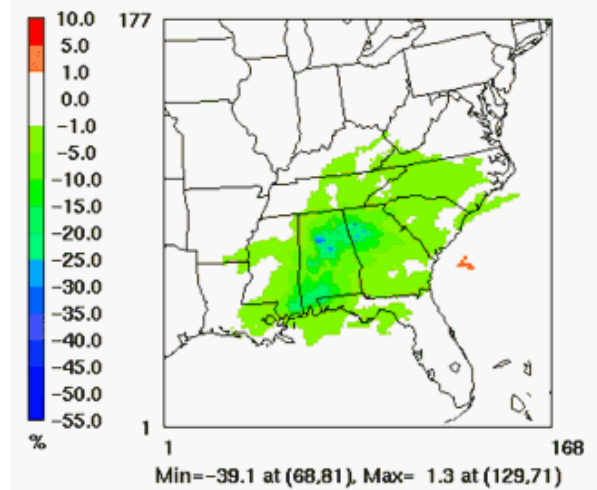


Absolute
Difference
(APT-Base)

PM_{2.5} Sulfate



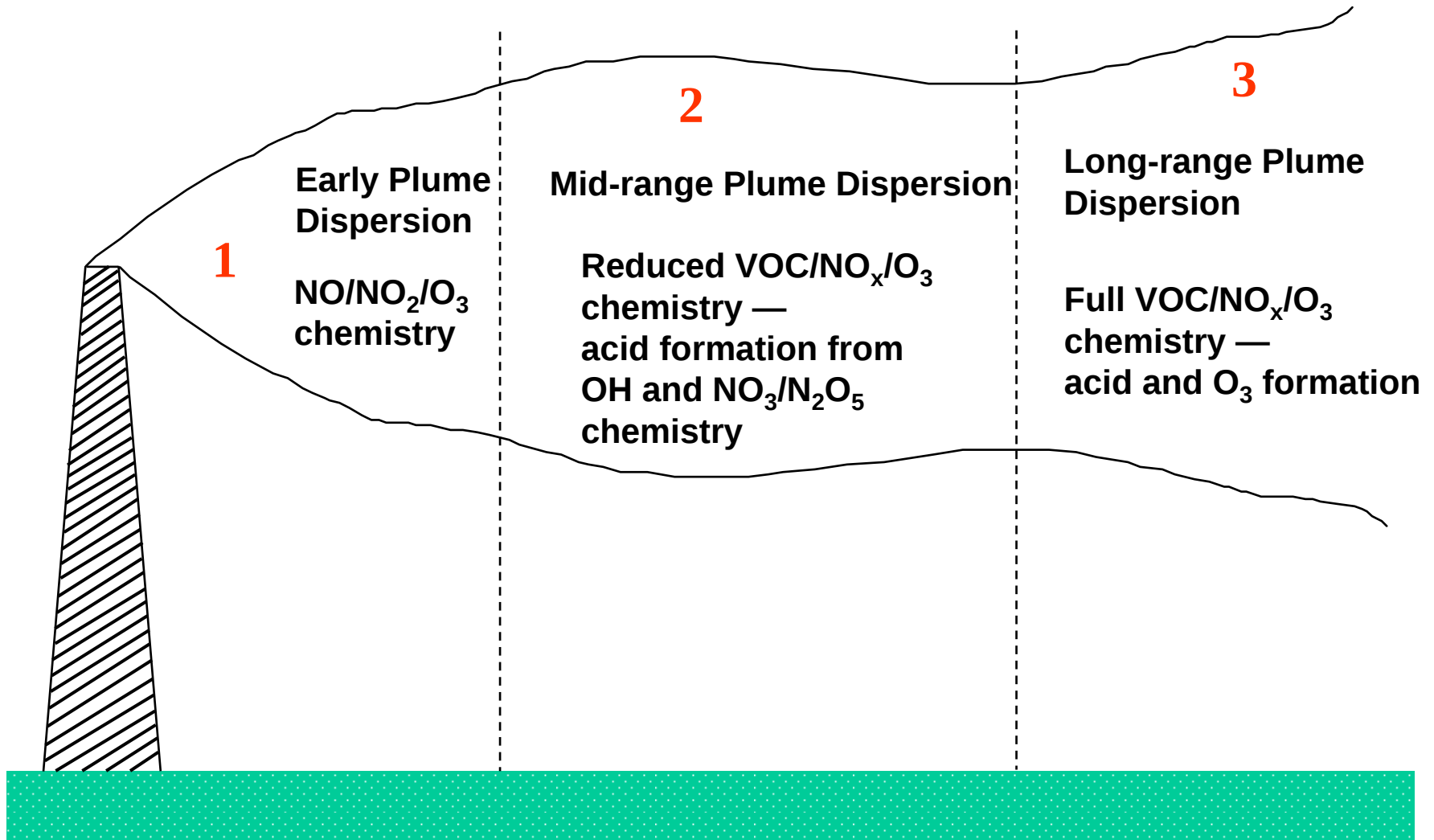
Percent
Difference





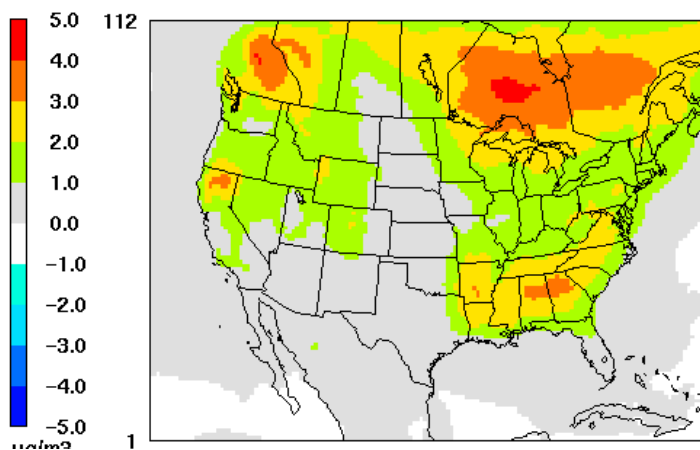
Plume Chemistry & Relevance to PM Modeling

(Karamchandani et al., 2005, 2006)

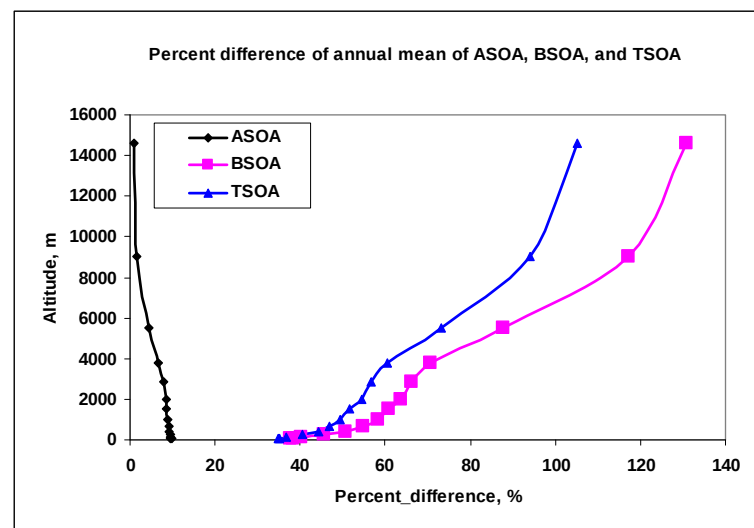


Contributions of Isoprene to Biogenic SOA in 2001

Summer (JJA)



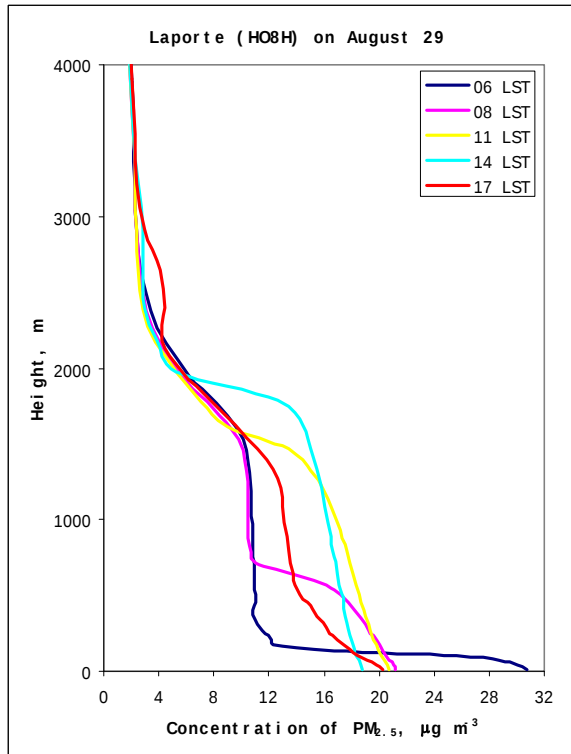
Annual



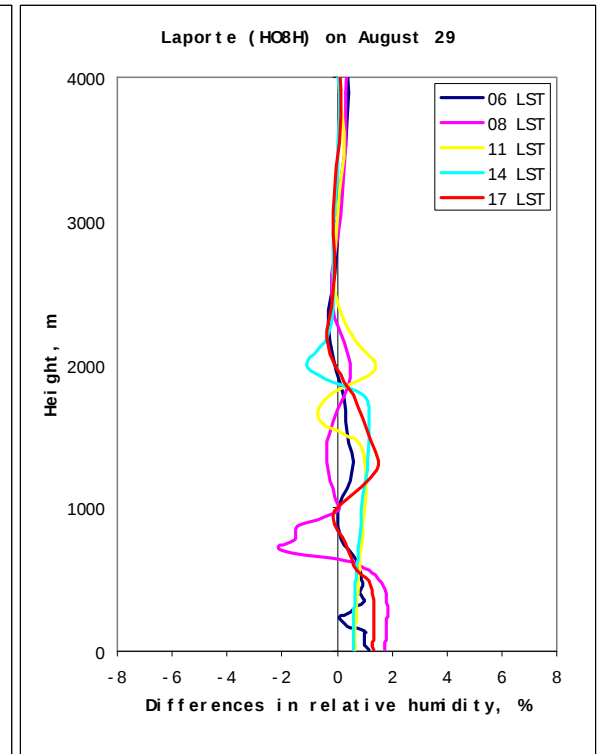
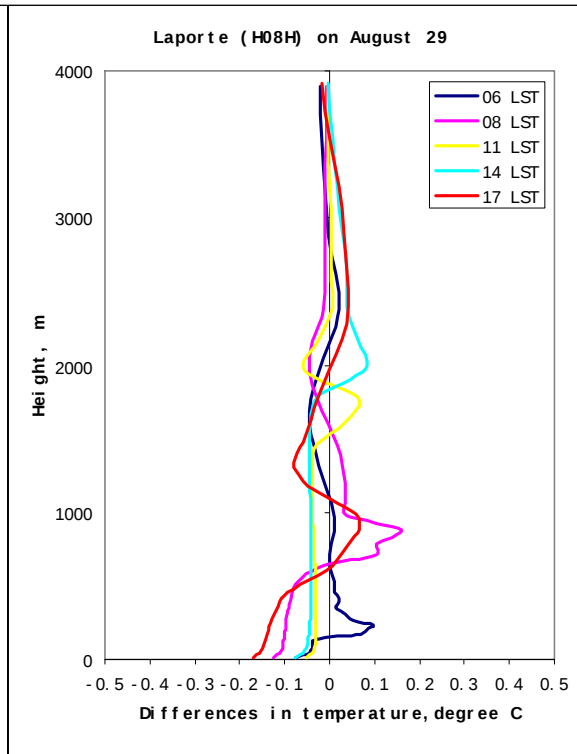
BSOA increases by $< 4.3 \mu\text{g m}^{-3}$ (up to 107%) in PBL (0-2.9 km)

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

PM_{2.5}



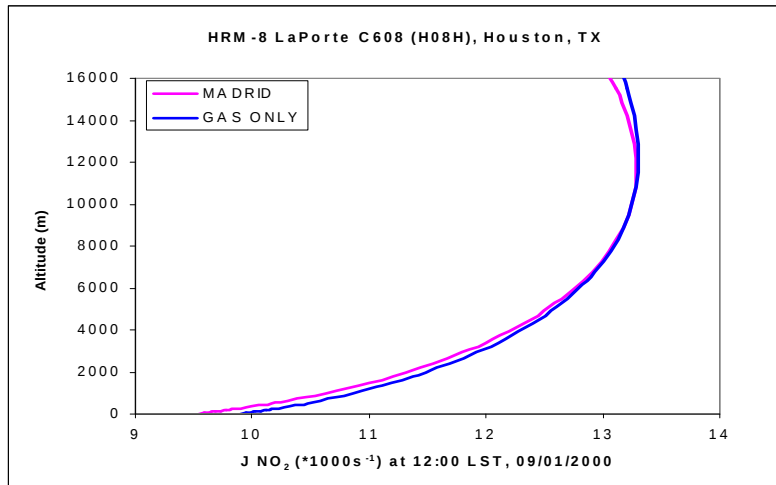
(Gas+PM - Gas only)



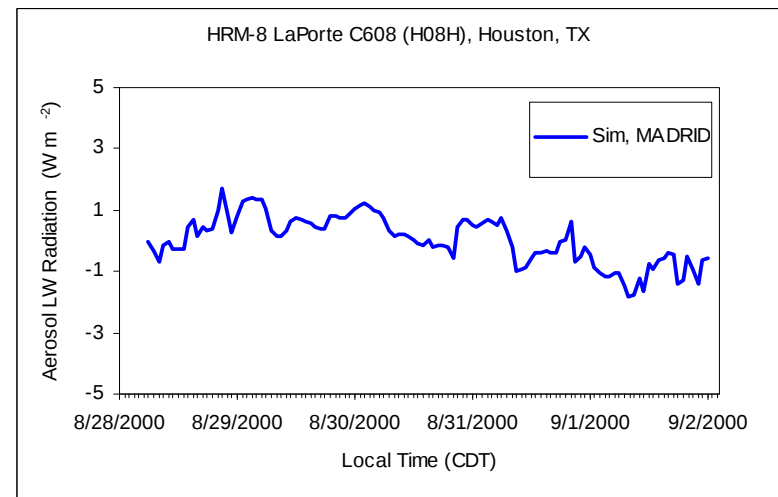
Diff > 0, T(RH) increases (decreases) due to aerosol feedbacks
Diff < 0, T(RH) decreases (increases) due to aerosol feedbacks

Feedbacks of Aerosols to NO_2 Photolysis and Radiative Forcing

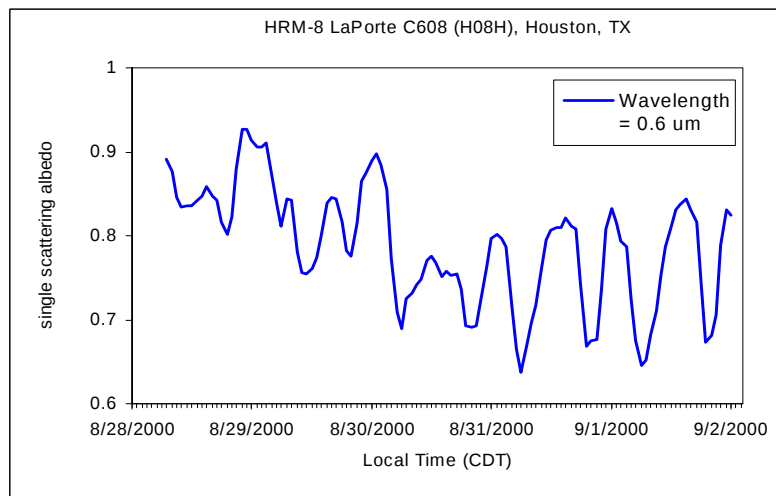
NO_2 Photolysis



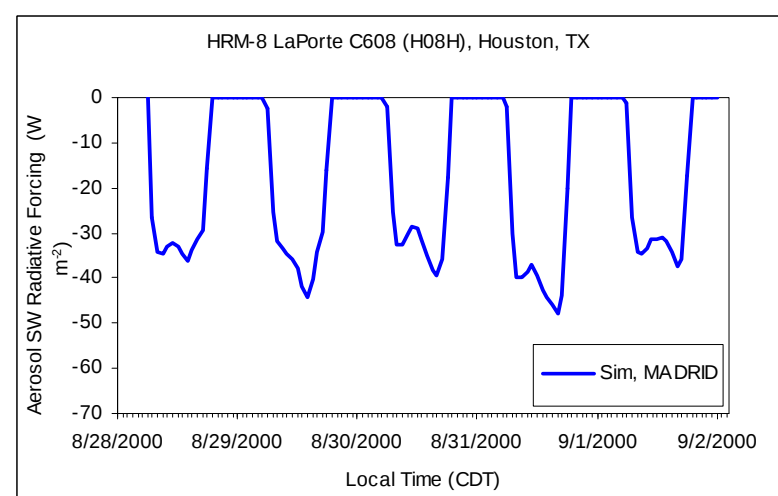
LW Radiative Forcing



Single Scattering Albedo

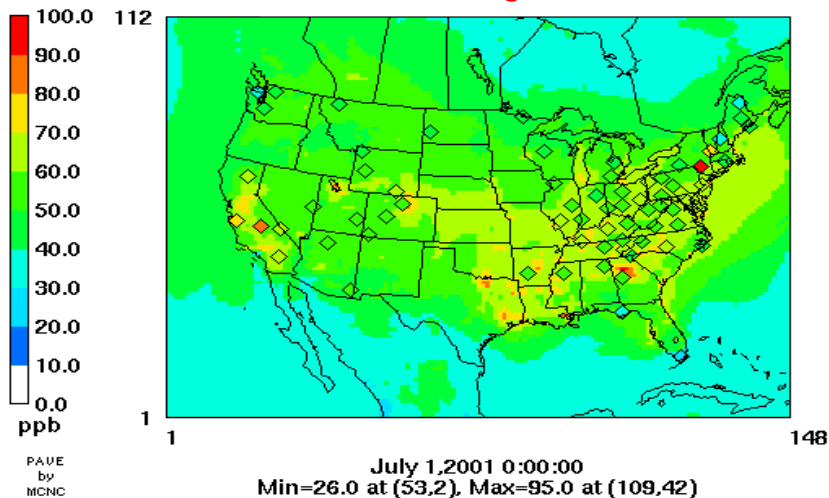


SW Radiative Forcing

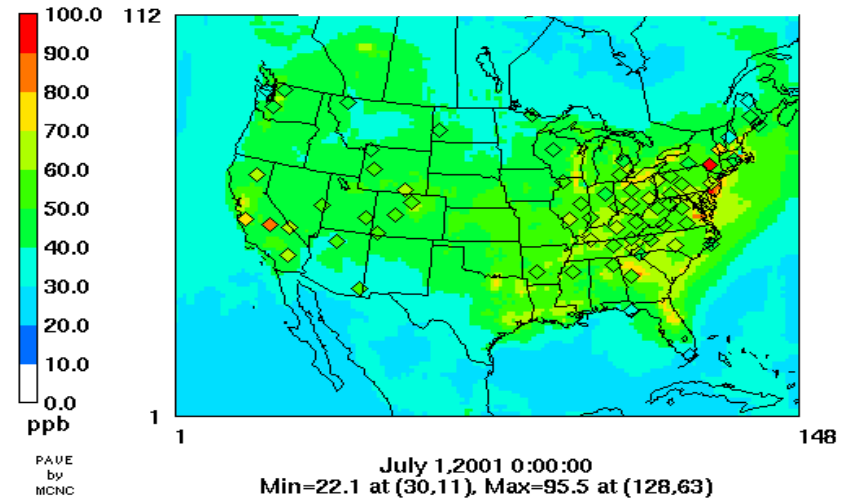


Weekly Mean Max 1-hr Average O₃ (CASTNet)

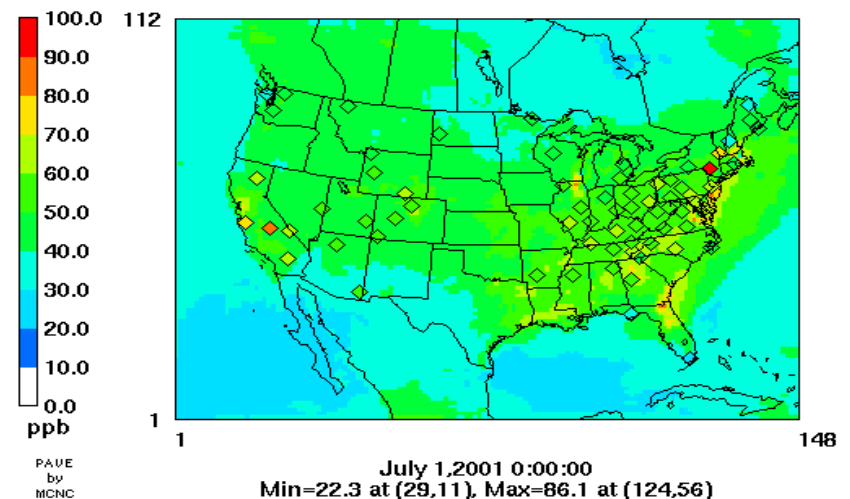
MM5/CMAQ-CB05



WRF/Chem-CB05



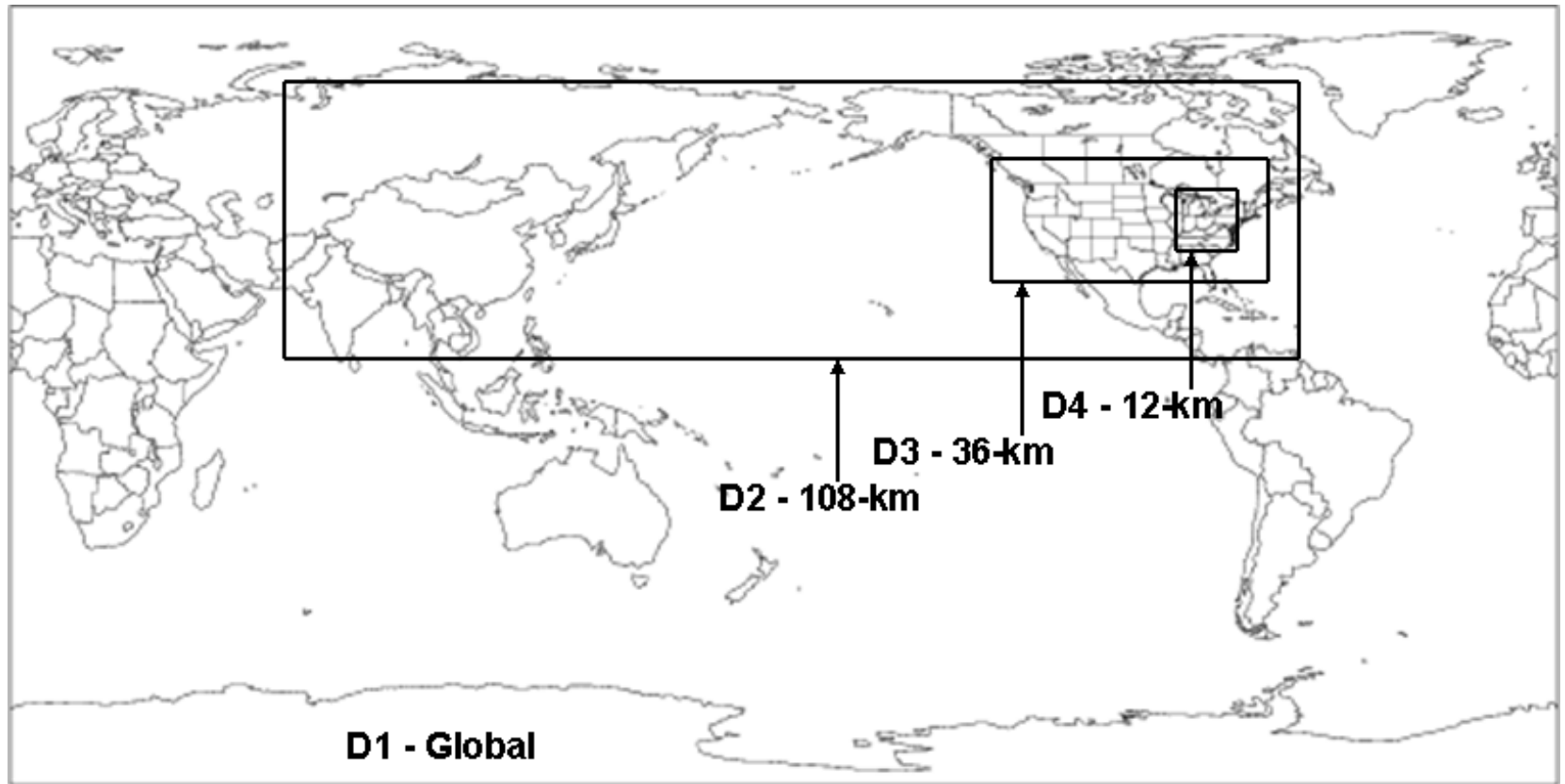
WRF/Chem-CBMZ



	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%

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, AVHRR, 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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- **John Seinfeld and Daven Henze, Caltech,** for providing isoprene SOA yield parameters based on their smog chamber data for incorporation into CMAQ
- **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						