Online Coupled Meteorology and Chemistry Models in the U.S.

Yang Zhang

North Carolina State University

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Outline

- Background
  - Important feedbacks between meteorology/climate and air quality
  - History and current status of online models
- Review of Several Online Models in the U.S.
  - GATOR/GCMOM Gas, Aerosol, TranspOrt, Radiation, General Circulation, Mesoscale, Ocean Model
  - WRF/Chem Weather Research and Forecast with Chem
  - CAM3 Community Atmospheric Model v. 3
  - MIRAGE2 Model for Integrated Research on Atmospheric Global Exchanges v. 2
- Applications of Online Models
  - GATOR/GCMOM
    - CA aerosol/climate modeling
  - WRF/Chem
    - CONUS and TeXAQS air quality
  - CAM3/MIRAGE
    - Global aerosol indirect effect
- Major Challenges and Future Directions

One Atmosphere

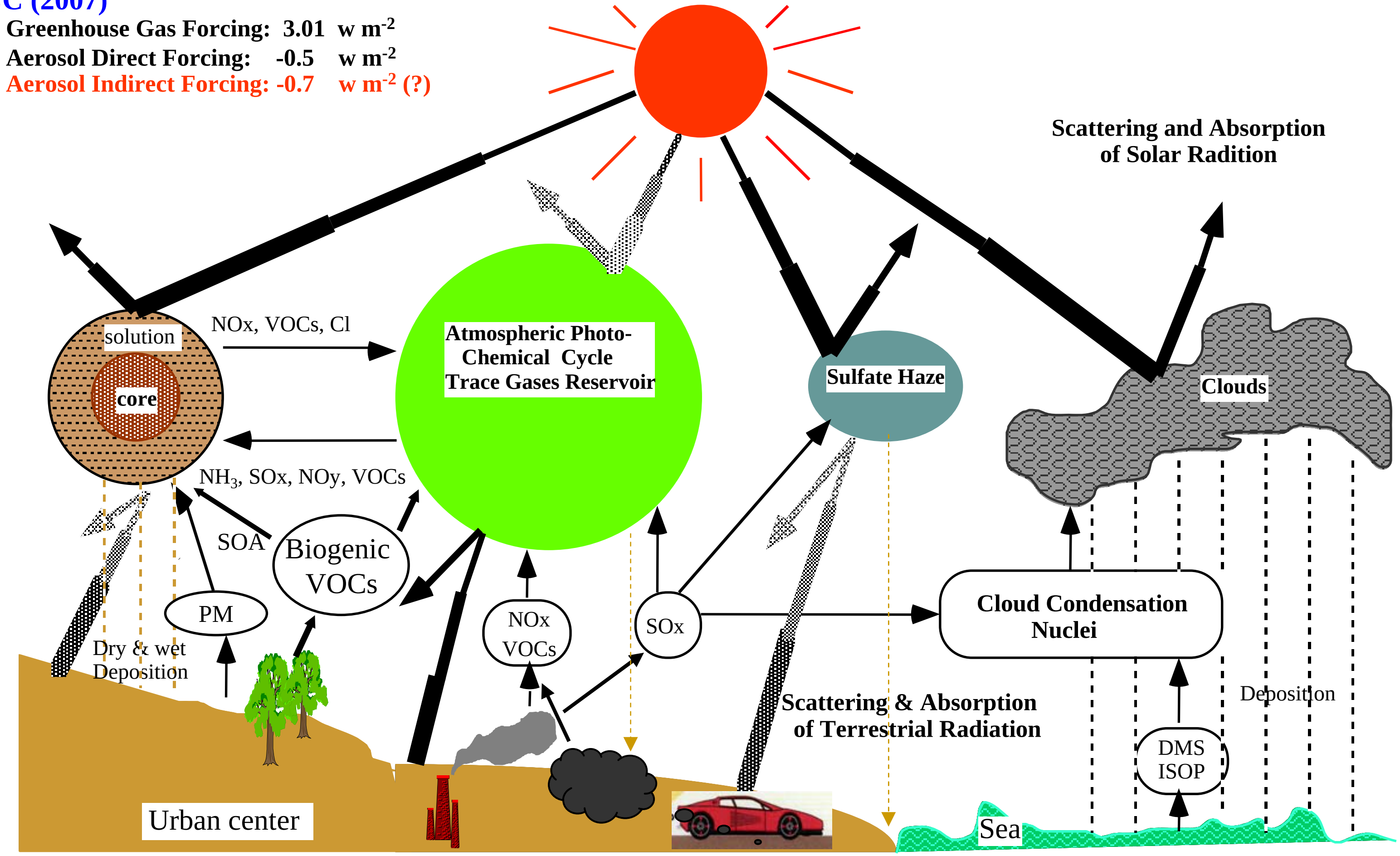
Gases, Aerosols, Chemistry, Transport, Radiation, Climate

IPCC (2007)

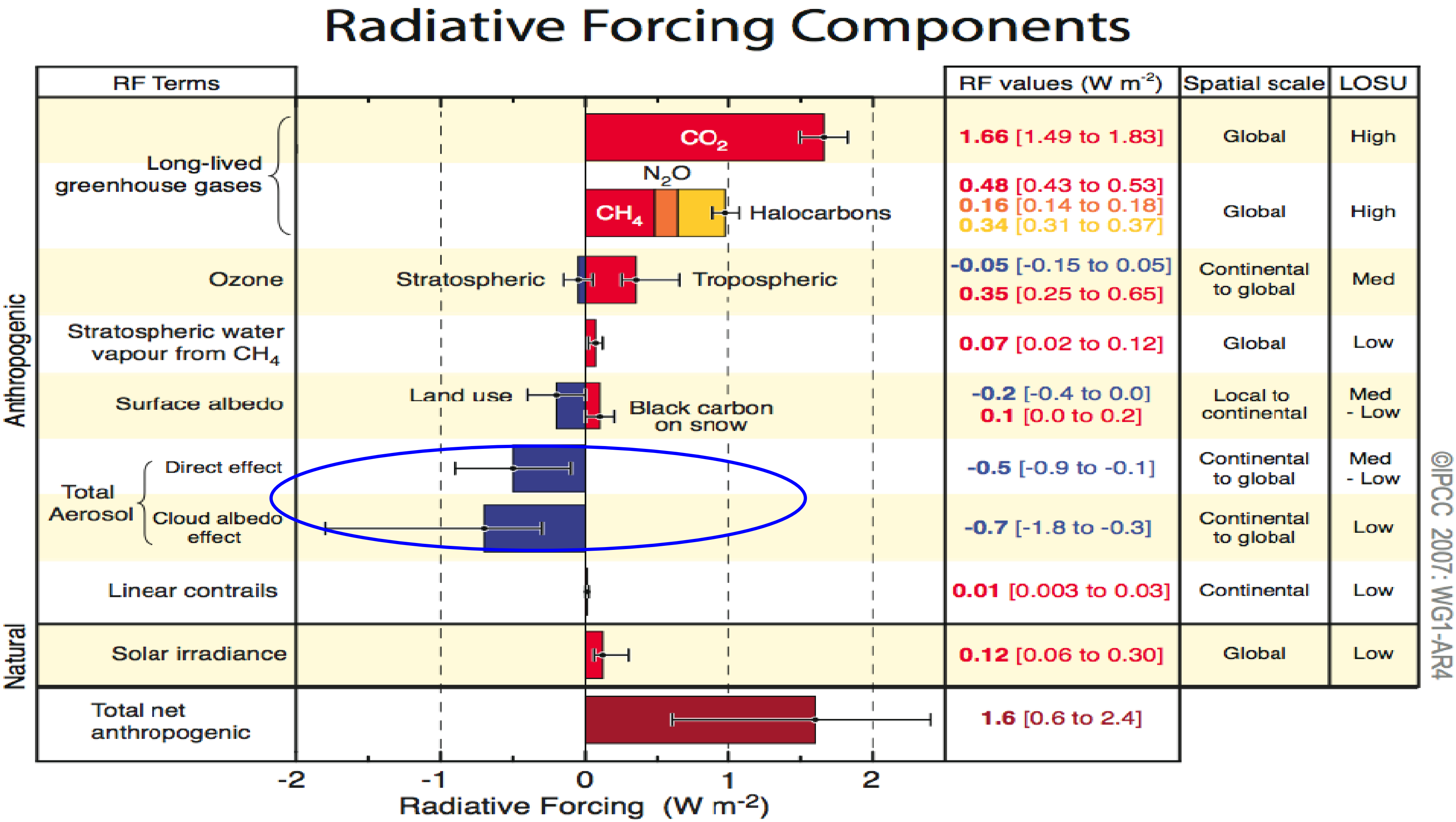
Greenhouse Gas Forcing: 3.01 w m^{-2}

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

Aerosol Indirect Forcing: -0.7 w m^{-2} (?)



2007 IPCC Estimate of Gas and Aerosol Radiative Effects



RF Terms		RF values (W m^{-2})	Spatial scale	LOSU
Long-lived greenhouse gases	CO$_2$	1.66 [1.49 to 1.83]	Global	High
	CH$_4$ N$_2$O Halocarbons	0.48 [0.43 to 0.53] 0.16 [0.14 to 0.18] 0.34 [0.31 to 0.37]	Global	High
Ozone	Stratospheric Tropospheric	-0.05 [-0.15 to 0.05] 0.35 [0.25 to 0.65]	Continental to global	Med
Stratospheric water vapour from CH$_4$		0.07 [0.02 to 0.12]	Global	Low
Surface albedo	Land use Black carbon on snow	-0.2 [-0.4 to 0.0] 0.1 [0.0 to 0.2]	Local to continental	Med - Low
Total Aerosol	Direct effect	-0.5 [-0.9 to -0.1]	Continental to global	Med - Low
	Cloud albedo effect	-0.7 [-1.8 to -0.3]	Continental to global	Low
Linear contrails		0.01 [0.003 to 0.03]	Continental	Low
Solar irradiance		0.12 [0.06 to 0.30]	Global	Low
Total net anthropogenic		1.6 [0.6 to 2.4]		

Examples of Important Feedbacks

- **Effects of Meteorology and Climate on Gases and Aerosols**
  - **Changes in temperature, humidity, and precipitation directly affect species conc.**
  - **The cooling of the stratosphere due to the accumulation of GHGs affects lifetimes**
  - **Changes in tropospheric vertical temperature structure affect transport of species**
  - **Changes in vegetation alter dry deposition and emission rates of biogenic species**
  - **Climate changes alter biological sources and sinks of radiatively active species**
- **Effects of Gases and Aerosols on Meteorology and Climate**
  - **Decrease net downward solar/thermal-IR radiation and photolysis (direct effect)**
  - **Affect PBL meteorology (decrease near-surface air temperature, wind speed, and cloud cover and increase RH and atmospheric stability) (semi-direct effect)**
  - **Aerosols serve as CCN, reduce drop size and increase drop number, reflectivity, and optical depth of low level clouds (LLC) (the Twomey or first indirect effect)**
  - **Aerosols increase liquid water content, fractional cloudiness, and lifetime of LLC but suppress precipitation (the second indirect effect)**

Coupling Air Quality and Meteorology/Climate Modeling

Rationale 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 meteorological 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 microphysics**

Coupling Air Quality and Meteorology/Climate Modeling

History and Current Status

- **Prior to 1994: Separation of air quality, meteorology, climate**
- **1994-Present: Offline and online coupling**
  - **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 chemistry and 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**

Fully Coupled Online Models

Model System and Application

Model System/Scale	Met. Model	Chemical Transport Model	Typical Applications	Example References
GATOR-GCMOM & Predecessors (Global-through-urban)	MMTD GCMM GCMOM	CBM-EX: (247 rxns, 115 species); size-resolved, prognostic aerosol/cloud with complex processes	Current/future met/ chem/rad feedbacks; Direct/indirect effects; AQ/health effect	Jacobson, 1994, 1997a, b, 2001, 2002, 2004; Jacobson et al., 2004, 2006, 2007
WRF/Chem (Mesoscale)	WRF	RADM2, RACM, CBMZ, CB05 (156-237 rxns, 52-77 species); Size/mode-resolved, prognostic aerosol/cloud	Forecast/hindcast, Met/chem feedbacks; O_3, $PM_{2.5}$; Aerosol direct effect	Grell et al. (2005), Fast et al. (2006), McQueen et al. (2005, 2007)
CAM3 & Predecessors (Global)	CCM3/ CCM2/ CCM1	Prescribed CH_4, N_2O, CFCs/MOZART4 (167 rxns, 63 species); Prognostic aerosol/cloud with prescribed size	Climate; Direct/indirect effects; Hydrological cycle	Collins et al., 2004, 2006; Rasch et al., 2006
MIRAGE2 & 1 (Global)	CAM2/ CCM2	CO-CH_4-oxidant chem.; Mode-resolved simple aerosol treatment; Prognostic aerosol/cloud	Trace gases and PM; Direct/indirect effects	Ghan et al., 2001a,b, Zhang et al., 2002; Easter et al., 2004;

Fully Coupled Online Models
Aerosol Properties

Model System	Composition	Size Distribution	Aerosol Mass/Number	Aerosol Mixing State
GATOR-GCMOM	47 species (sulfate, nitrate, ammonium, BC, OC, sea-salt, dust, crustal)	Sectional (17-30): variable, multiple size distributions	Predicted/Predicted	A coated core, internal/external mixtures
WRF/ Chem	Sulfate, nitrate, ammonium, BC, OC, sea-salt	Modal (3): variable (MADE/SORGAM) Sectional (8): variable (MOSAIC/MADRID) single size distribution	Predicted/Diagnosed from mass or predicted	Internal
CAM3	Sulfate, nitrate, ammonium, BC, OC, sea-salt, dust	Modal (4): predicted dust and sea-salt, prescribed other aerosols; single size distribution	Prescribed or predicted/Diagnosed from mass	External
MIRAGE2	Sulfate, BC, OC, sea-salt, dust	Modal (4): variable; single size distribution	Prescribed or predicted/Diagnosed or predicted	Externally mixed modes with internal mixtures within each mode

Fully Coupled Online Models

Aerosol/Cloud Properties

Model System	Aerosol Hygroscopicity	Aerosol radiative properties	Cloud droplet number	Hydrometeor types in clouds
GATOR-GCMOM	Simulated hydrophobic-to-hydrophilic conversion for all aerosol components	Simulated volume-average refractive indices and optical properties based on core-shell MIE theory	Prognostic, size- and composition-dependent from multiple aerosol size distributions	Size-resolved liquid, ice, graupel, aerosol core components
WRF/ Chem	The same as MIRAGE2	The same as MIRAGE2	The same as MIRAGE2 (MOSAIC)	Bulk single condensate
CAM3	simulated hydrophobic and hydrophilic BC/OC with a fixed conversion rate	Prescribed RI and optical properties, for external mixtures	The same as MIRAGE2	Bulk liquid, ice water
MIRAGE2	Simulated BC/OC with prescribed hygroscopicities	Parameterized RI and optical properties based on wet radius and RI of each mode	Prognostic, size- and composition-dependent, parameterized	Bulk single condensate

Fully Coupled Online Models

Cloud Properties

Model System	Cloud droplet size distri.	CCN/IDN composition	CCN/IDN spectrum	Cloud radiative properties
GATOR-GCMOM	Prognostic, sectional (30), multiple size distributions (3)	All types of aerosols treated for both CCN/IDN	Predicted with Köhler theory; sectional (13-17); multiple size distributions (1-16) for both CCN/IDN	Simulated volume-average refractive indices and optical properties based on MIE theory and a dynamic effective medium approximation
WRF/ Chem	Prognostic, sectional, single size distribution (MOSAIC)	The same as MIRAGE2 but sectional; CCN only	The same as MIRAGE2 but sectional, CCN only	The same as MIRAGE2 but sectional (MOSAIC)
CAM3	The same as MIRAGE2	All treated species except hydrophobic species; CCN only	Prescribed; CCN only	The same as MIRAGE2
MIRAGE2	Prescribed, modal, single size distribution	All treated species; CCN only	Function of aerosol size and hygroscopicity based on Köhler theory; CCN only	Prognostic, parameterized in terms of cloud water, ice mass, and number

Fully Coupled Online Models
Aerosol Chemistry and Microphysics

Model System	Inorganic aero. thermo-dyn. equili.	Secondary organic aero. formation	New Particle Formation	Condensation of Gases on aerosols
GATOR-GCMOM	EQUISOLV II, major inorganic salts and crustal species	Condensation; Dissolution based on Henry's law (10-40 classes VOCs)	Binary homogeneous nucleation of H_2SO_4 and H_2O, T- and RH-dependent	Dynamic condensation of all condensible species based on growth law (e.g., H_2SO_4, VOCs)
WRF/ Chem	MARS-A (SORGAM) MESA-MTEM (MOSAIC) ISORROPIA (MADRID)	Reversible absorption (8 classes VOCs) based on smog-chamber data	Binary homogeneous nucleation of H_2SO_4 and H_2O; T- and RH-dependent; sectional; different eqs. in different aero module	Dynamic condensation of H_2SO_4 and VOCs (SORGAM), H_2SO_4 and MSA(MOSAIC), and inorganic species (MADRID)
CAM3	MOZART4 with regime equili. for sulfate, ammonium and nitrate	Prescribed SOA yield for α-pinene, n-butane, and toluene	None	Instantaneous condensation of inorganic species
MIRAGE2	Simple equilibrium involving $(NH_4)_2SO_4$ and precursor gases	Prescribed SOA yield	Binary homogeneous nucleation of H_2SO_4 and H_2O; T- and RH-dependent	Dynamic condensation of H_2SO_4 and MSA based on Fuchs and Sutugin growth law

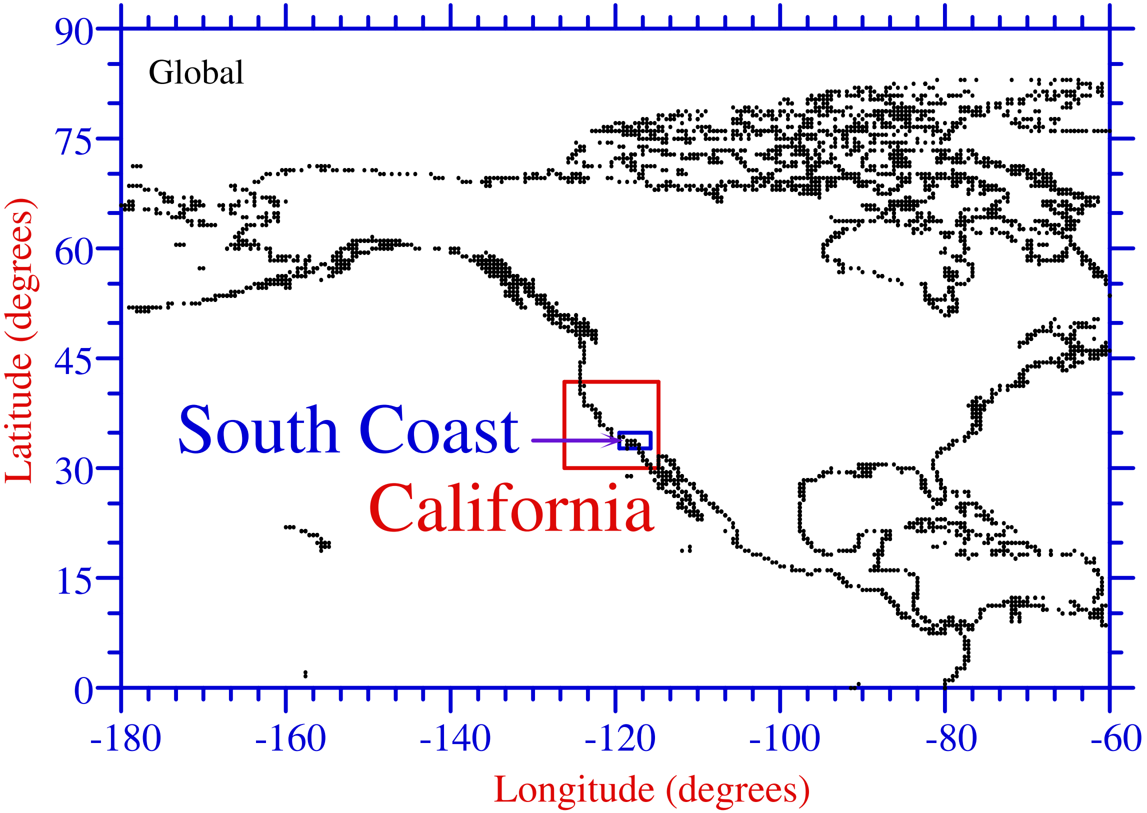
Fully Coupled Online Models
Aerosol Chemistry and Microphysics

Model System	Coagulation	Gas/particle mass transfer	Aqueous chemistry	Aerosol activation aero-CCN/IDN
GATOR-GCMOM	Sectional, multiple size distributions, accounts for van der Waals and viscous forces, and fractal geometry	Dynamic approach with a long time step (150-300 s) (PNG-EQUISOLV II) for all treated species	Bulk or size-resolved sulfate, nitrate, organics, chlorine, oxidant, radical chemistry (64 kinetic rxns)	Mechanistic, size- and composition-resolved CCN/IDN based on Köhler theory
WRF/ Chem	Modal/Sectional, single size distribution, fine-mode only	1. Full equili. 2. Dynamic 3. Hybrid	Bulk RADM chemistry (MADE/SORGAM) Bulk CMU mechanism (MOSAIC/MADRID)	The same as MIRAGE2 but sectional (MOSAIC)
CAM3	None	Full equilibrium involving $(NH_4)_2SO_4$ and NH_4NO_3	Bulk sulfate chemistry (3 kinetic rxns)	Empirical, prescribed activated mass fraction; bulk CCN only
MIRAGE	Modal, single size distribution, fine-mode only	Simple equilibrium involving $(NH_4)_2SO_4$ and precursor gases	Bulk sulfate chemistry (3 kinetic rxns)	Mechanistic, parameterized activation based on Köhler theory; bulk CCN only

Fully Coupled Online Models
Aerosol/Cloud Microphysics

Model System	Water uptake	In-cloud Scavenging	Below-cloud Scavenging	Droplet Sedimentation
GATOR-GCMOM	Equilibrium with RH; ZSR equation; simulated MDRH; Hysteresis is treated	Aerosol activation Nucl. Scavenging (rainout) precip. rate dependent of aerosol size and composition	Aerosol-hydrometeor coag. (washout), precip. rate dependent of aerosol size and composition	size-dependent sedimentation
WRF/ Chem	The same as MIRAGE2 but sectional	The same as MIRAGE2 but sectional	The same as MIRAGE2 but sectional	The same as MIRAGE2
CAM3	For external mixtures only, equilibrium with RH, no hysteresis	Prescribed activation, autoconversion, precip. rate independent of aerosols	Prescribed scav. efficiency, no-size dependence	size-dependent sedimentation
MIRAGE2	Equilibrium with RH, Hysteresis is treated	Activation, Brownian diffusion (inters./activated), autoconversion, nucleation scavenging, precip. rate independent of aerosols	Prescribed scavenging efficiency with size dependence	no droplet sedimentation

GATOR/GCMOM: Nested Model Grids
(courtesy by Mark Jacobson, Stanford University)



California Climate Modeling

Baseline

Feb./Aug., 1999 Gas+PM

Sensitivity

Remove all anthropogenic aerosol and precursor gas emissions (AAPPG)

Removed emissions

BC, OC, sulfate, nitrate, dust

SO_x, NO_x, NH_3, ROGs

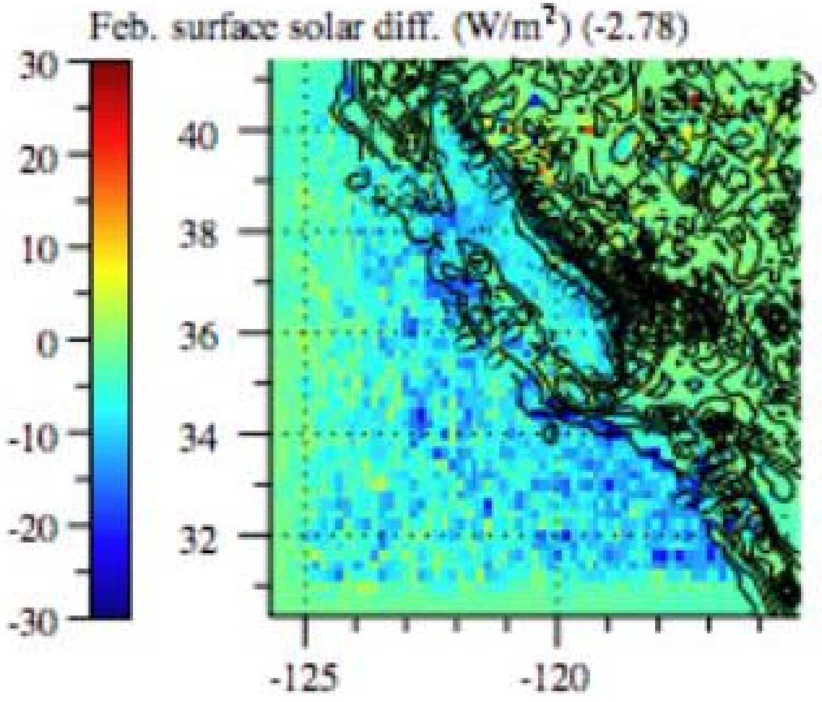
Global Grid: 4˚-SN × 5˚-WE

California Grid: 0.2˚ × 0.15˚, ~21.5 km × 14.0 km

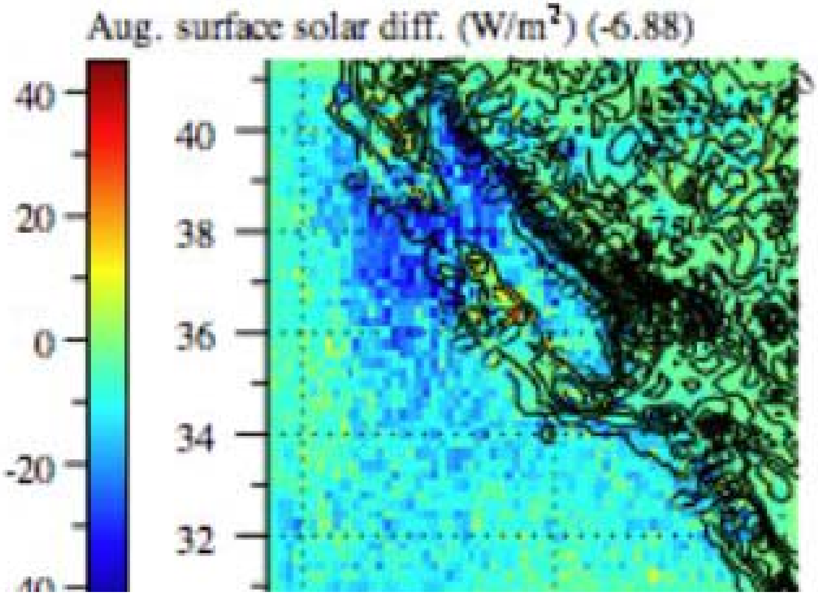
South Coast Air Basin Grid: 0.045˚ × 0.05˚, ~4.7 km × 5 km

Feb. and Aug. Down-Up Surface Solar Radiation Dif. w-w/o AAPPG

(courtesy by Mark Jacobson, Stanford University)



Feb. surface solar diff. (W/m²) (-2.78)

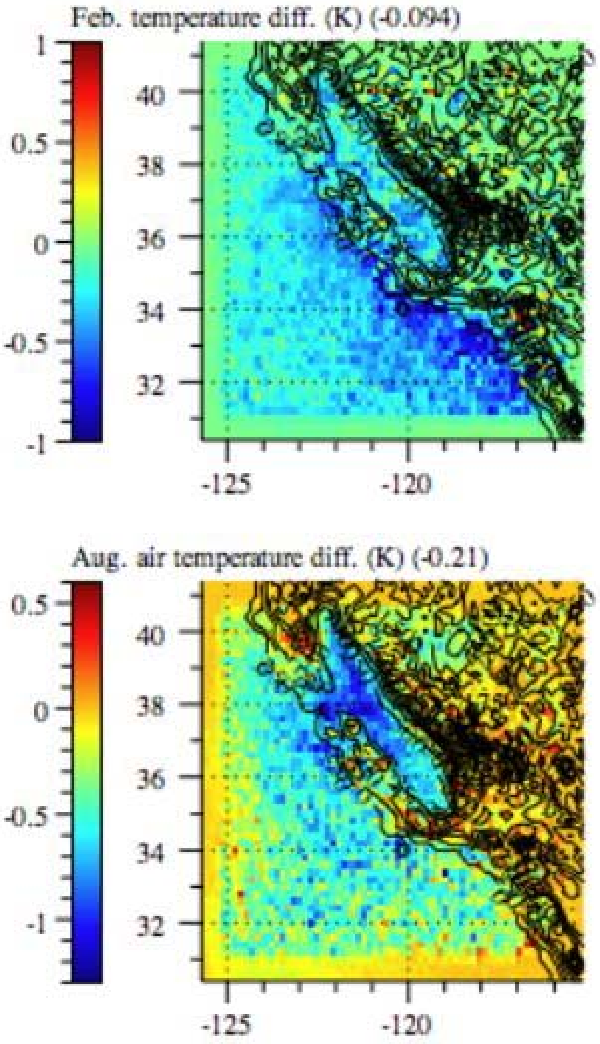


Aug. surface solar diff. (W/m²) (-6.88)

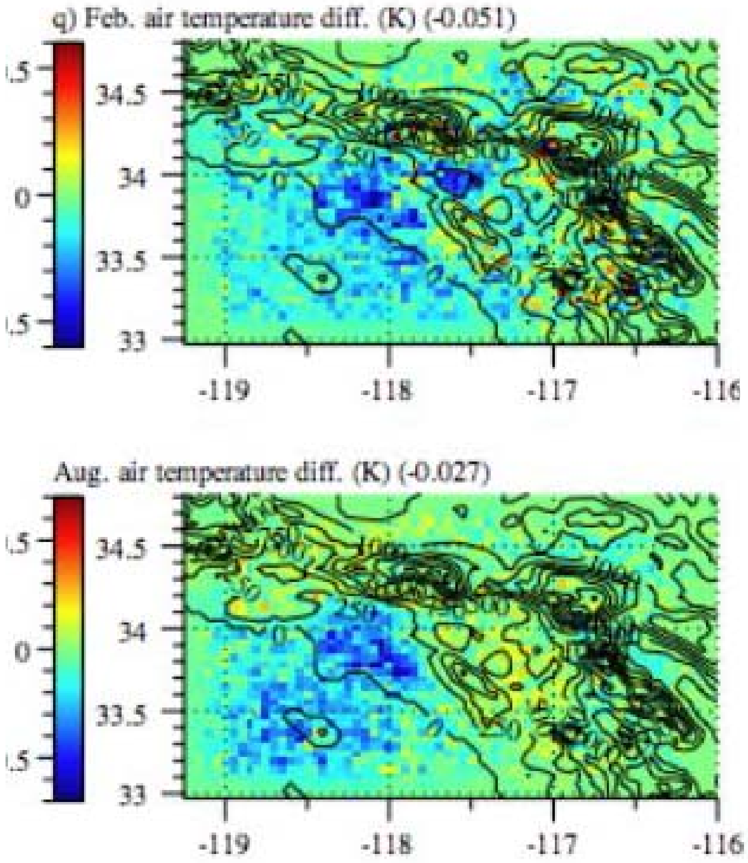
Aerosols decrease surface solar radiation

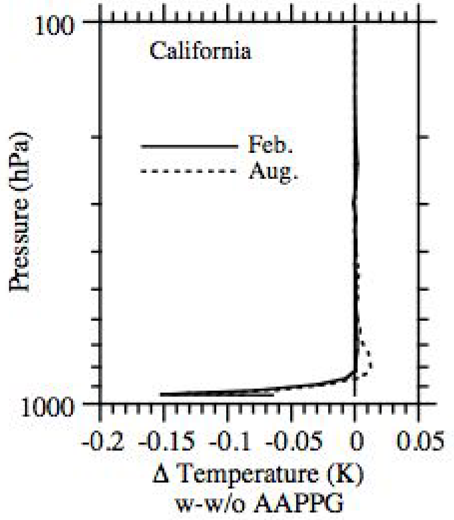
Feb. and Aug. Temperature Differences w-w/o AAPPG
(courtesy by Mark Jacobson, Stanford University)

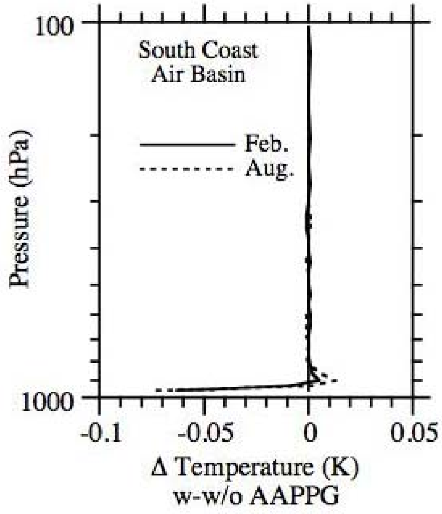
California



South Coast, CA

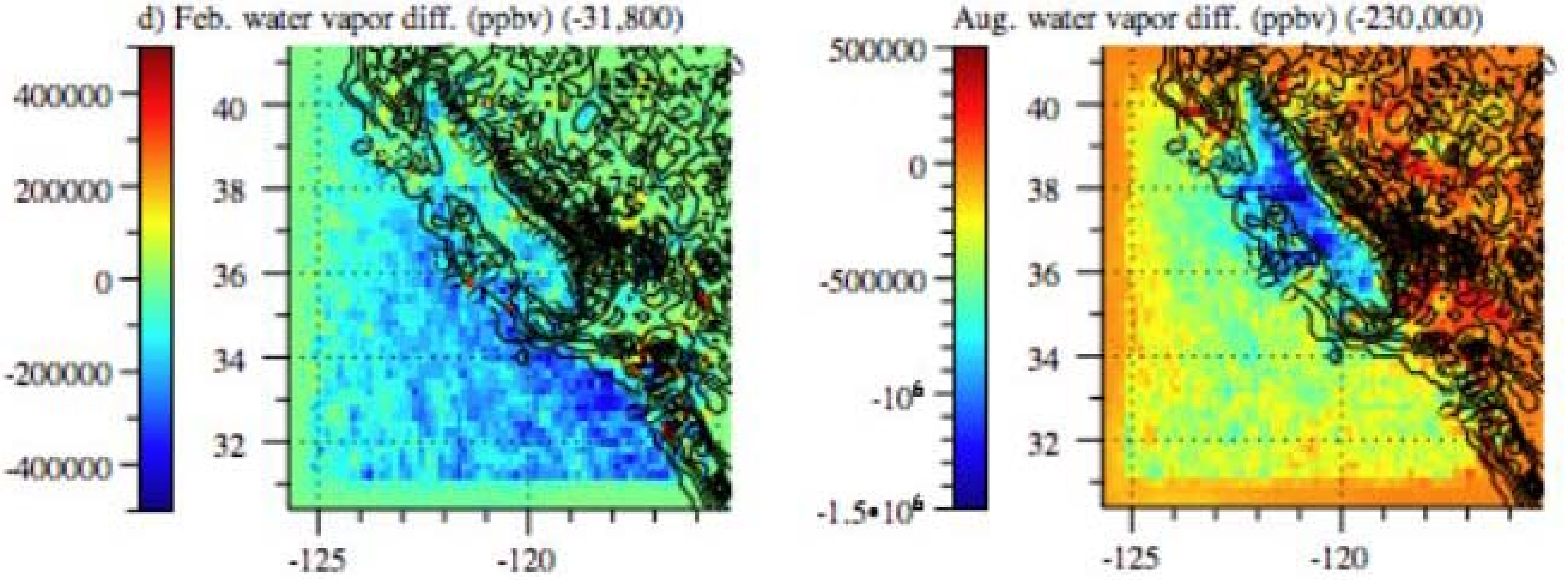






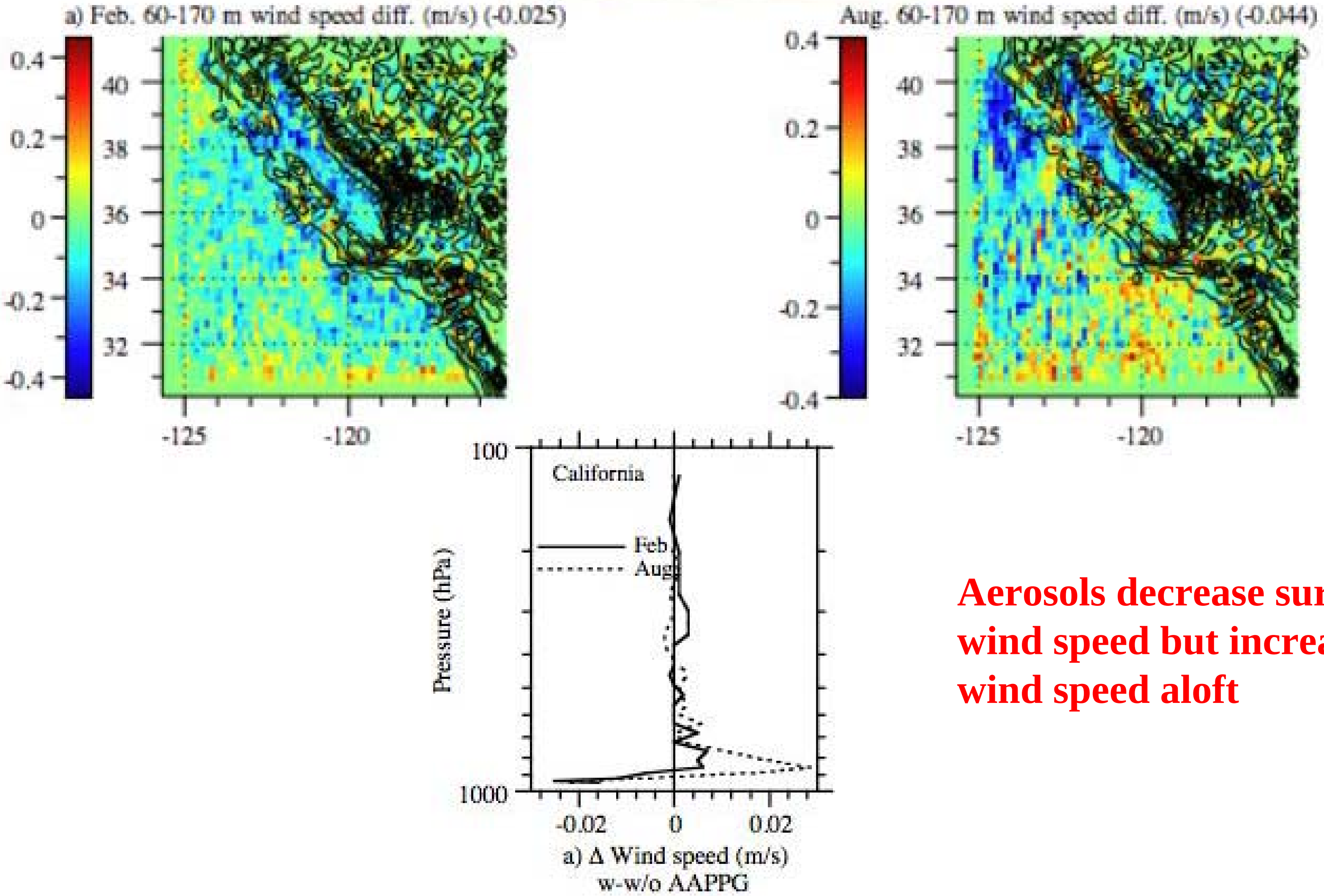
Aerosols decrease surface temp.
but increase boundary-layer temp.

Feb. and Aug. Water Vapor Differences w-w/o AAPPG (courtesy by Mark Jacobson, Stanford University)



Cooling and stability due to aerosols suppress evaporation

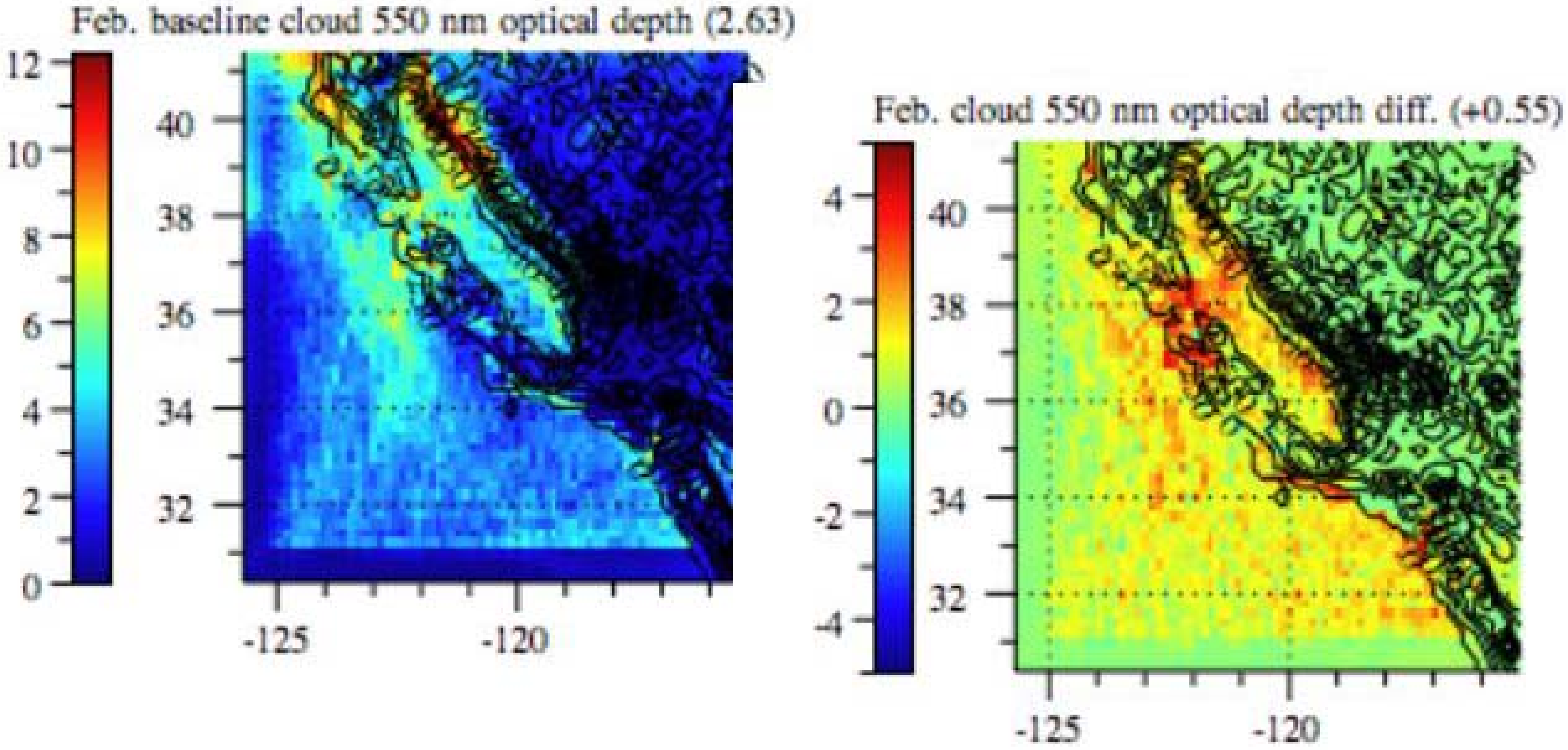
Feb. and Aug. 60-170 Wind Speed Differences w-w/o AAPPG
(courtesy by Mark Jacobson, Stanford University)



Aerosols decrease surface wind speed but increase wind speed aloft

Modeled Feb. Cloud Optical Depth Base and Diff. w-w/o AAPPG

(Courtesy by Mark Jacobson, Stanford University)



Aerosols increase cloud optical depths

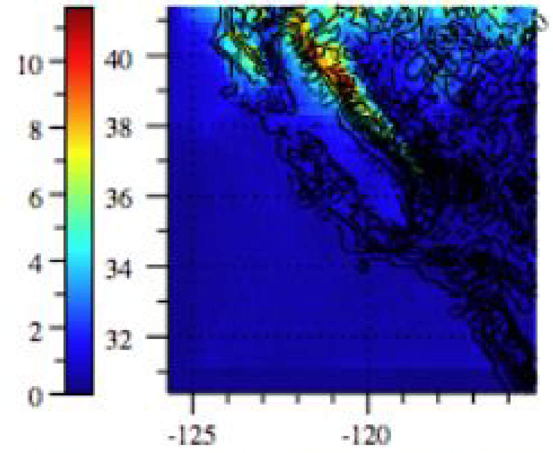
Feb. Precipitation Baseline and Differences
(courtesy by Mark Jacobson, Stanford University)

California

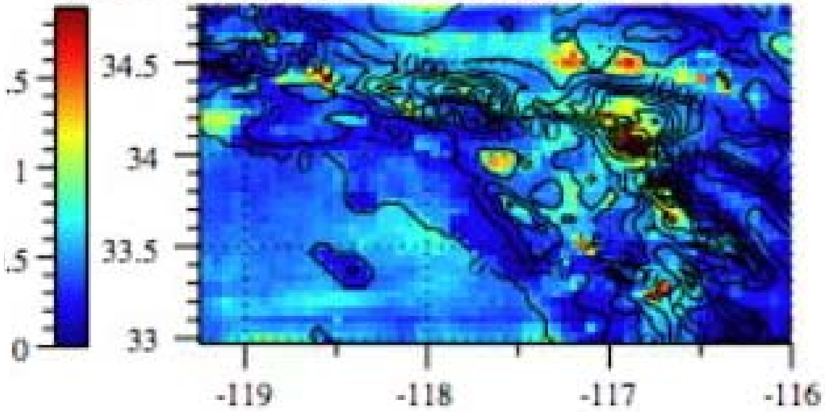
South Coast, CA

Baseline

Feb. baseline precipitation (mm/day) (1.55)

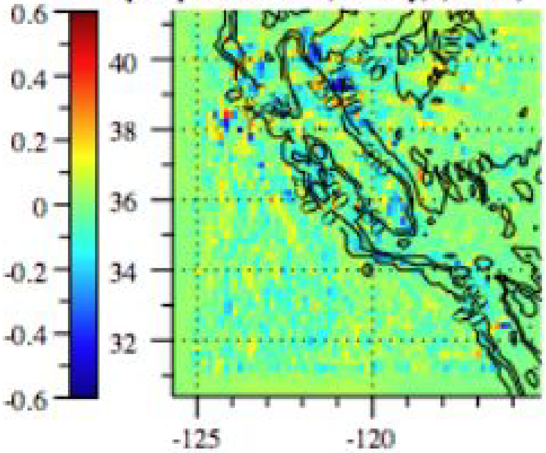


r) Feb. baseline precipitation (mm/day) (0.50)

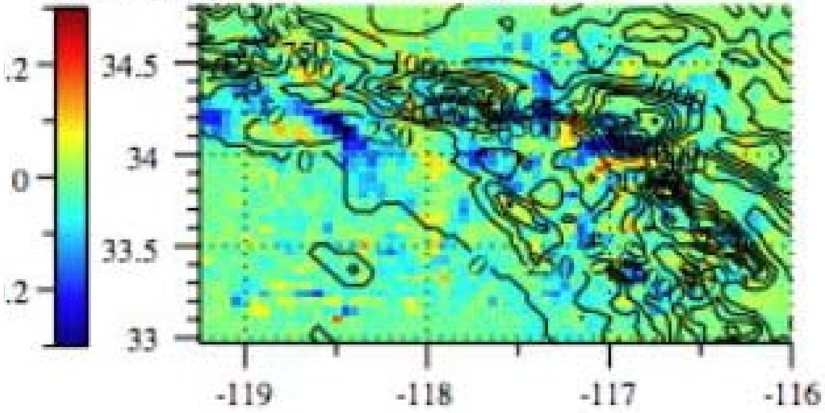


Difference (w-w/o AAPPG)

Feb. precipitation diff. (mm/day) (-0.026)



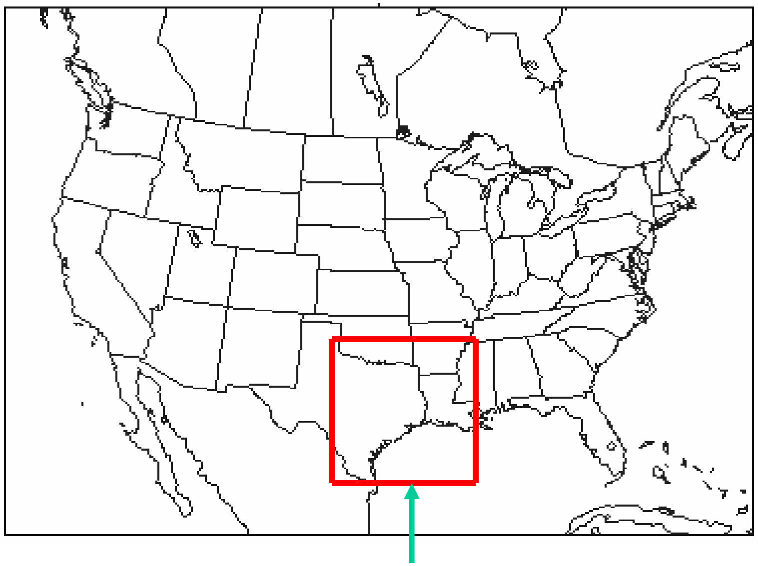
t) Feb. precipitation diff. (mm/day) (-0.029)



Aerosols decrease precipitation

WRF/Chem-MADRID
Model Configurations

July 1-7 2001 CONUS



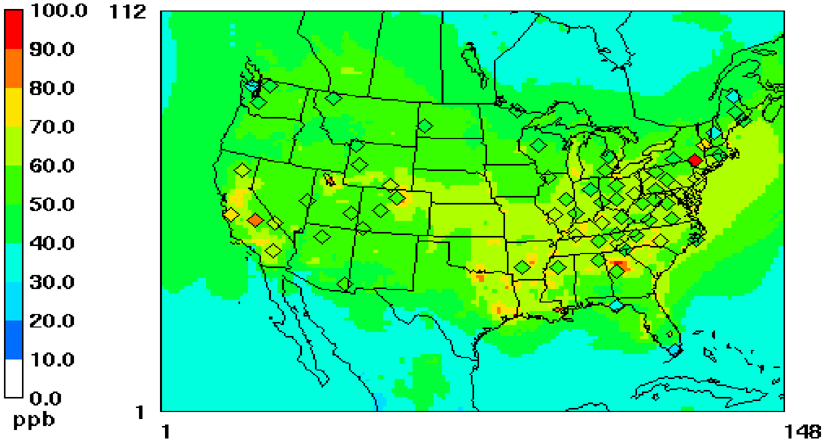
- Horizontal resolution: 36 km (148 × 112)
- Vertical resolution:
  - MM5 (L34), CMAQ (L14)
  - WRF/Chem (L34)
- Emissions:
  - SMOKE: US EPA NEI'99 (v3)
- Initial and boundary conditions:
  - The same ICs/BCs for WRF/ MM5 and for CMAQ and WRF/Chem
- Gas-phase chemical mechanism:
  - CMAQ: CB05
  - WRF/Chem: CB05 or CBMZ
- Data for model evaluation:
  - CASTNet and SEARCH

Aug. 28-Sept. 2, 2000 TeXAQS

- Horizontal resolution: 12 km (88 × 88)
- Vertical grid spacing: L57, 15-m at L1
- Emissions
  - Gases from TCEQ
  - PM based on EPA's NEI'99 V. 3 + online s.s.
- Initial/boundary conditions
  - 3-hr N. Amer. reg. reanal. for met.
  - Horizontally homogeneous ICs
- Gas-phase chemical mechanism: CBMZ
- Data for model evaluation
  - CASTNet, IMPROVE, AIRS, STN, TeXAQS

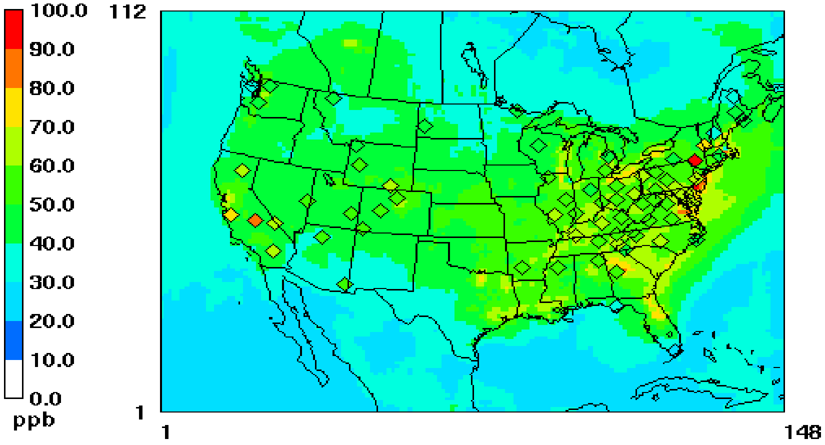
Offline MM5/CMAQ vs. Online WRF/Chem
Differences in Meteorology and Gas-Phase Chemistry

MM5/CMAQ-CB05



July 1,2001 0:00:00
Min=26.0 at (53,2), Max=95.0 at (109,42)

WRF/Chem-CB05

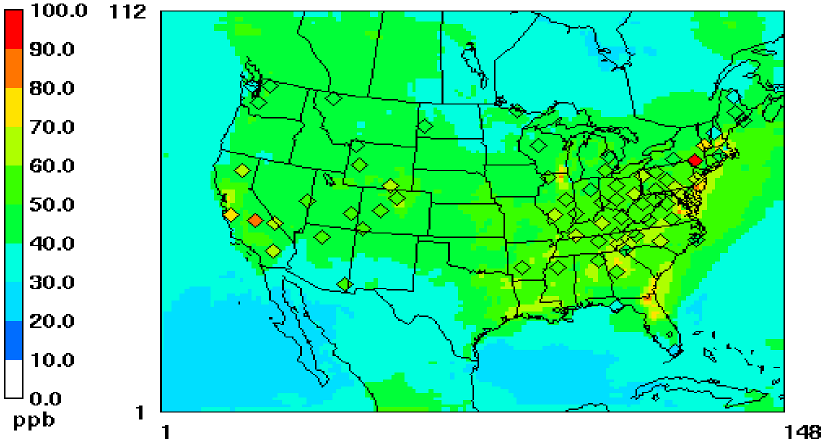


July 1,2001 0:00:00
Min=22.1 at (30,11), Max=95.5 at (128,63)

Weekly Mean Max 1-hr Average O3 (CASTNet)

	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

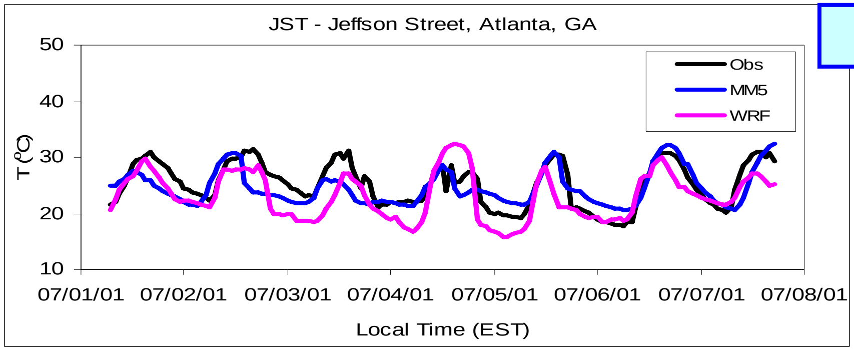


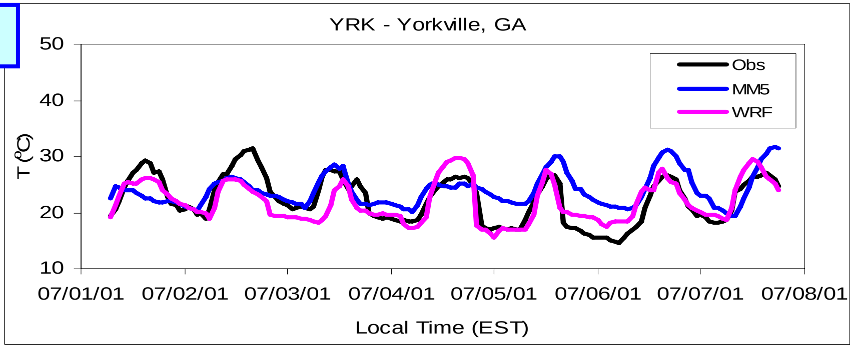
July 1,2001 0:00:00
Min=22.3 at (29,11), Max=86.1 at (124,56)

Simulated vs. Observed Meteorological Variables

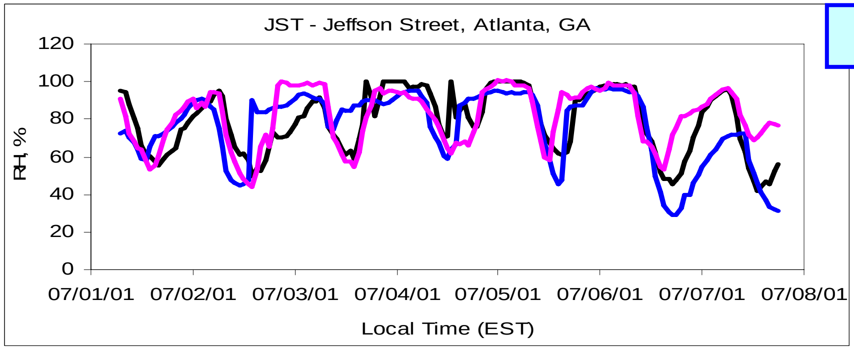
JST (Urban) YRK (Rural)

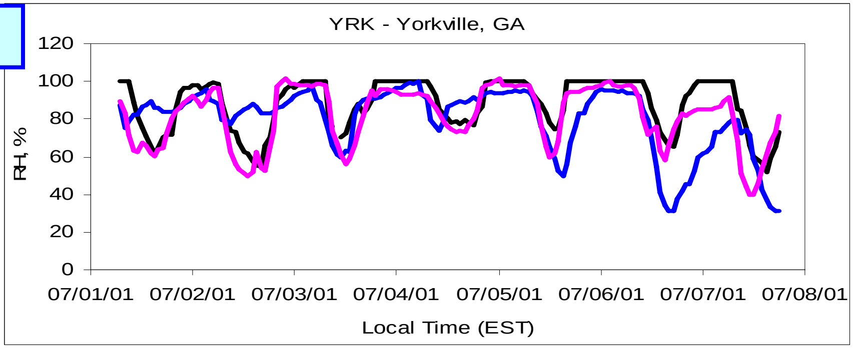
T



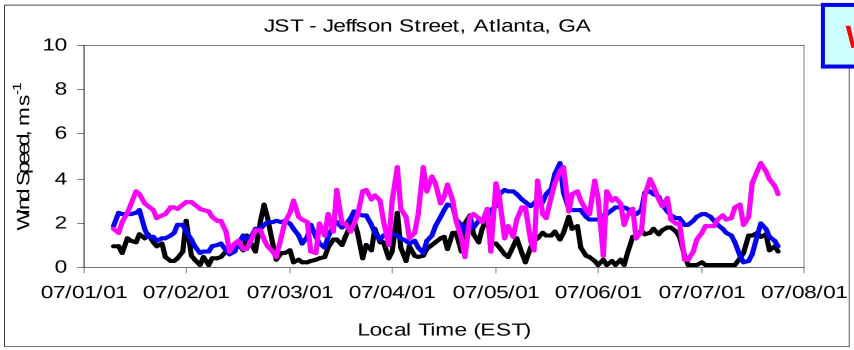


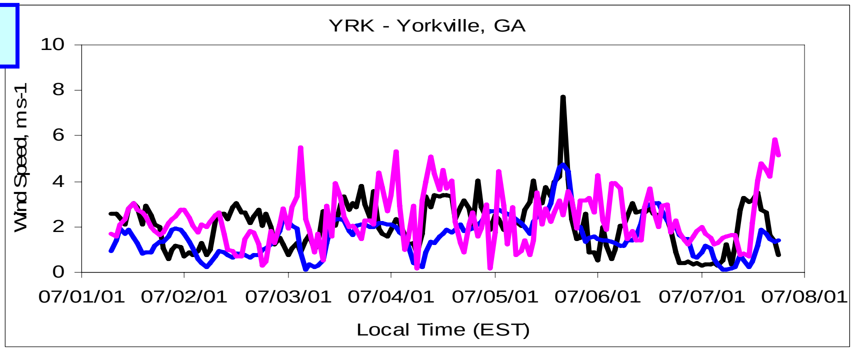
RH





WSP

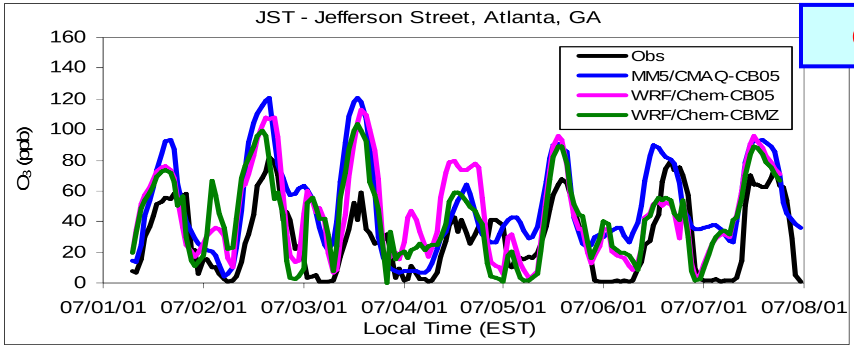


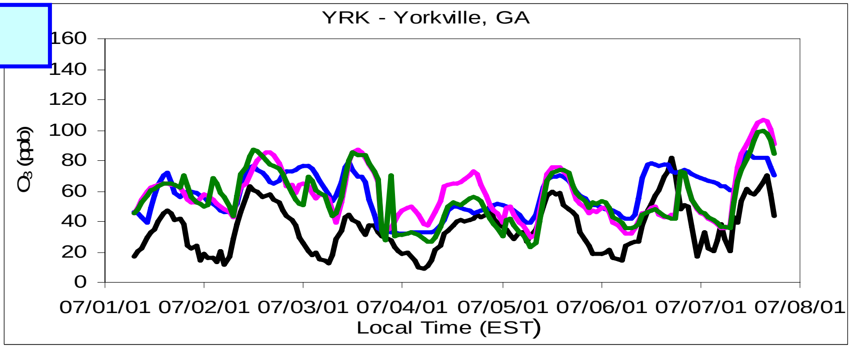


Simulated vs. Observed Mixing Ratios

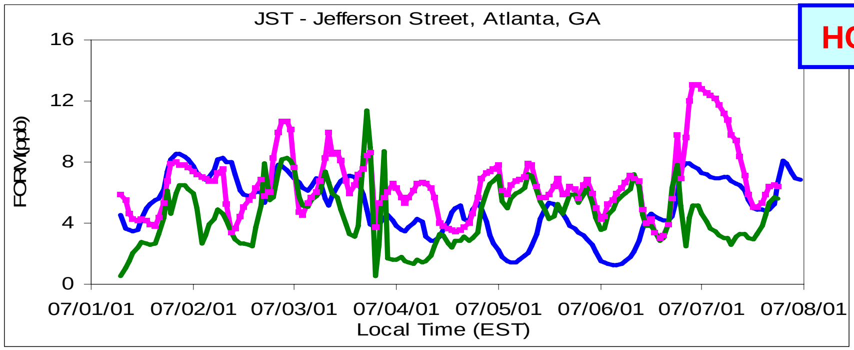
JST (Urban) YRK (Rural)

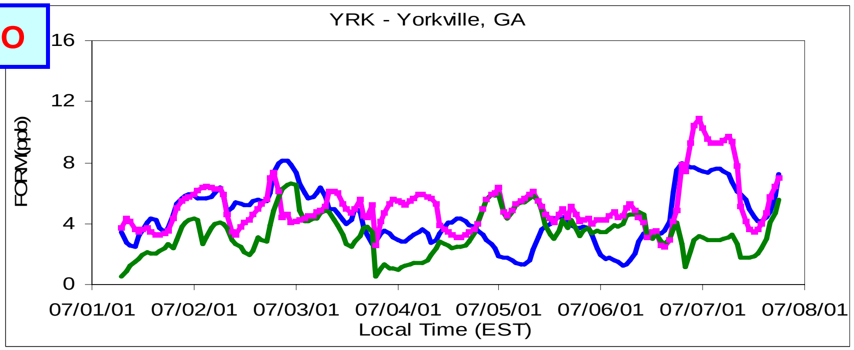
O_3



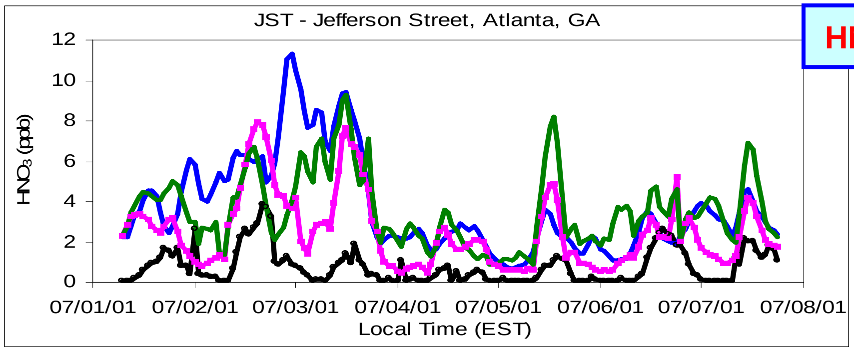


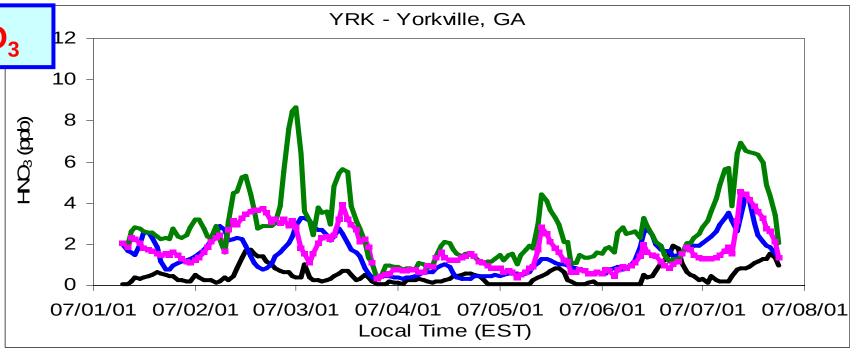
HCHO





HNO_3

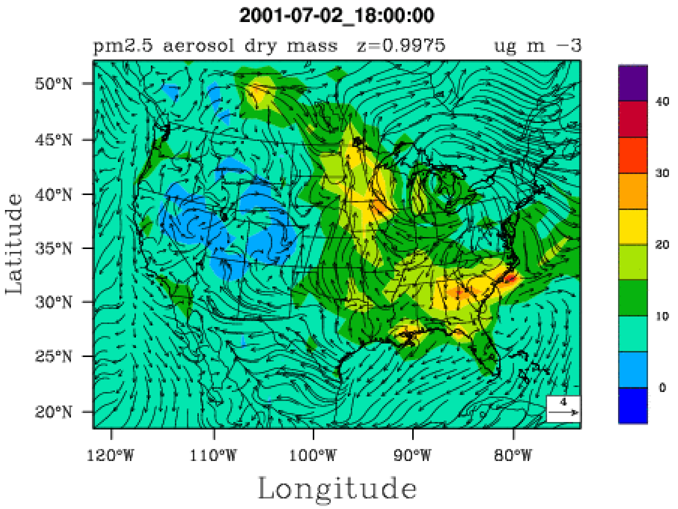


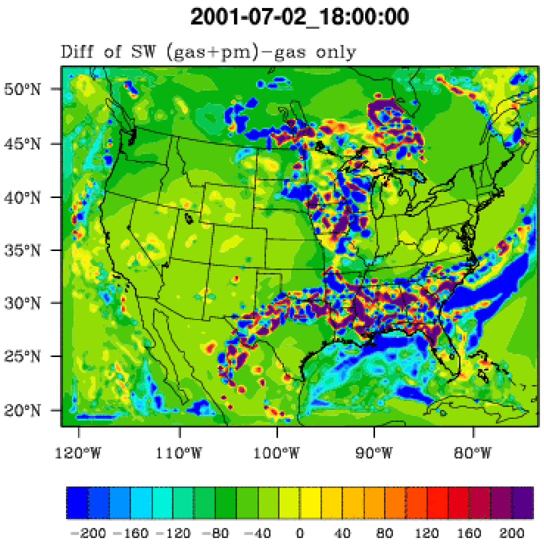


WRF/Chem-MADRID-CBMZ

Effects of Aerosols on Meteorology and Radiation

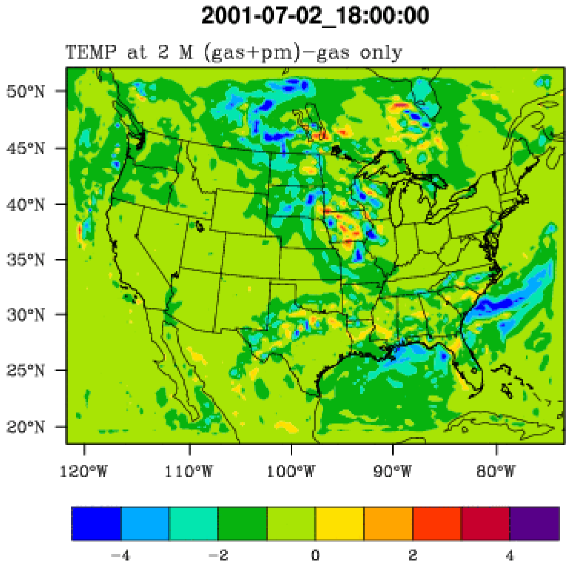
PM2.5

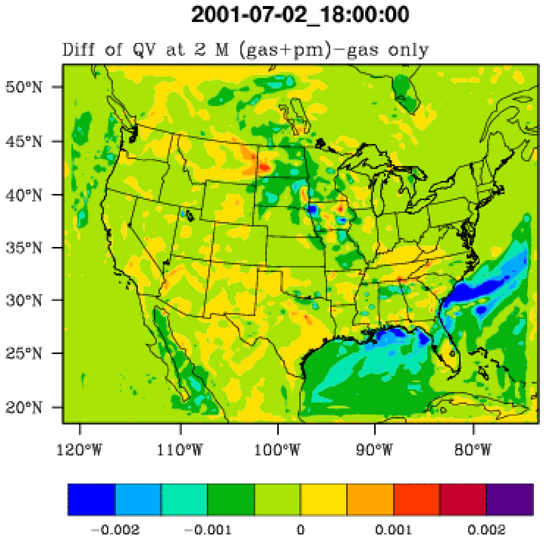




SW Radiation (-20 to 20%)

2-m Temp (-20% to 10%)





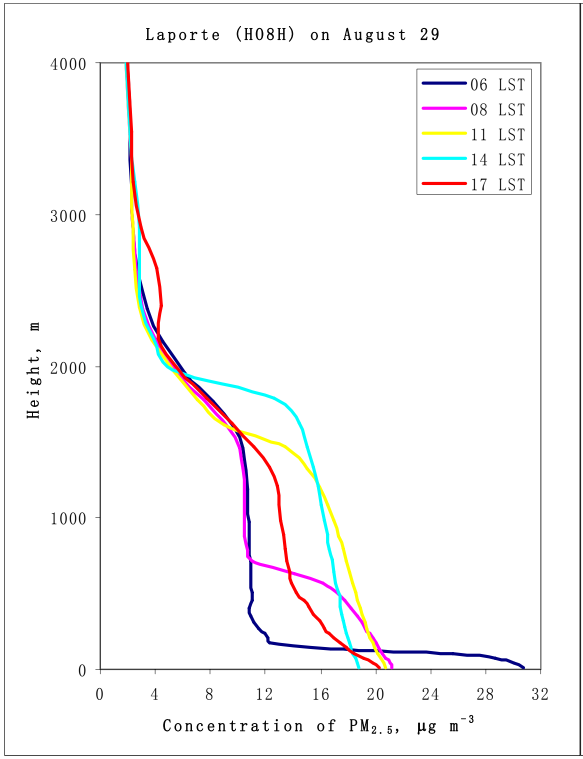
2-m Water Vapor (-10% to 10%)

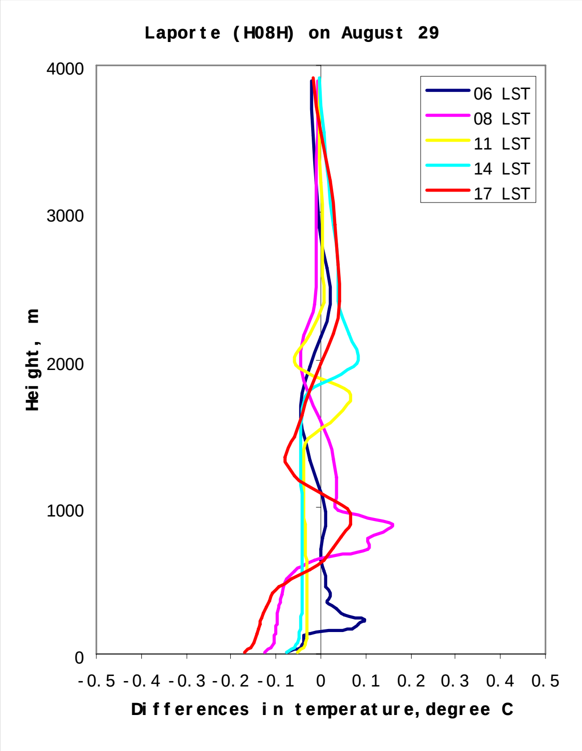
WRF/Chem-MADRID-CBMZ

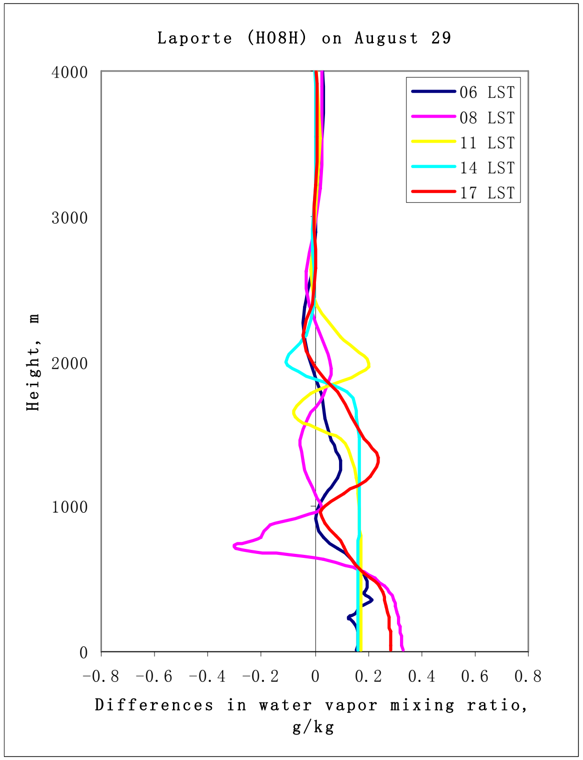
Feedbacks of Aerosols to T and Q_v at LaPorte, TX

$PM_{2.5}$

(Gas+PM - Gas only)







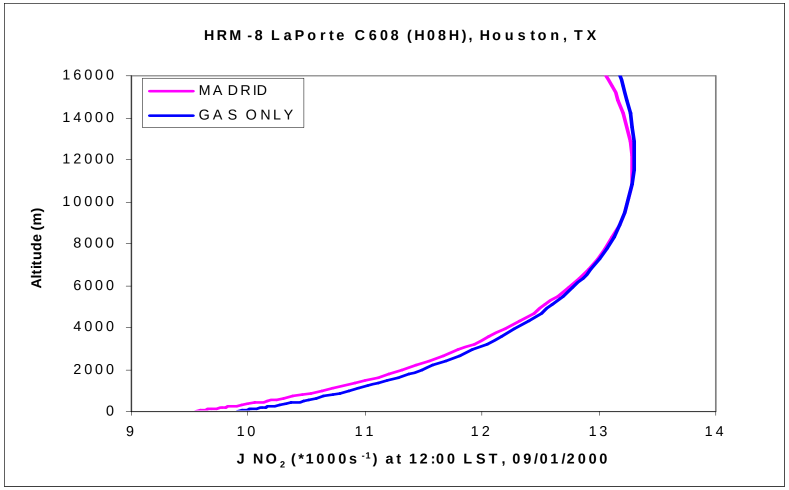
Diff > 0, T(Q_v) increases (decreases) due to aerosol feedbacks

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

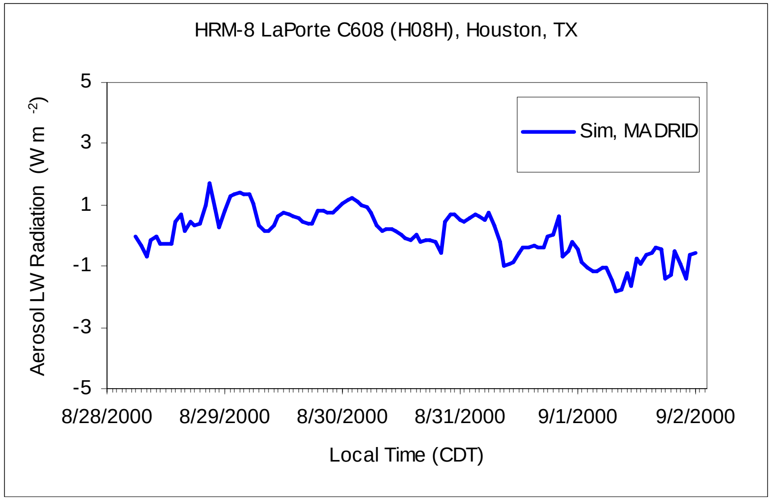
WRF/Chem-MADRID-CBMZ

Feedbacks of Aerosols to NO_2 Photolysis and Radiation

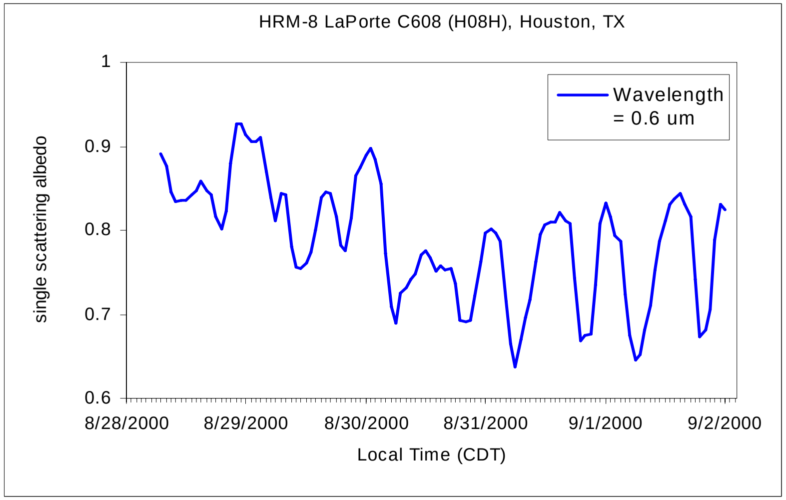
NO_2 Photolysis



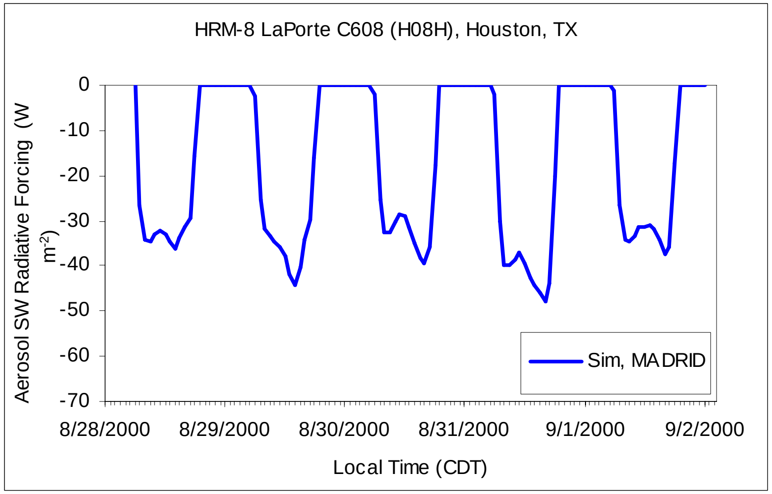
LW Radiative Forcing



Single Scattering Albedo



SW Radiative Forcing



CAM3 vs. MIRAGE2

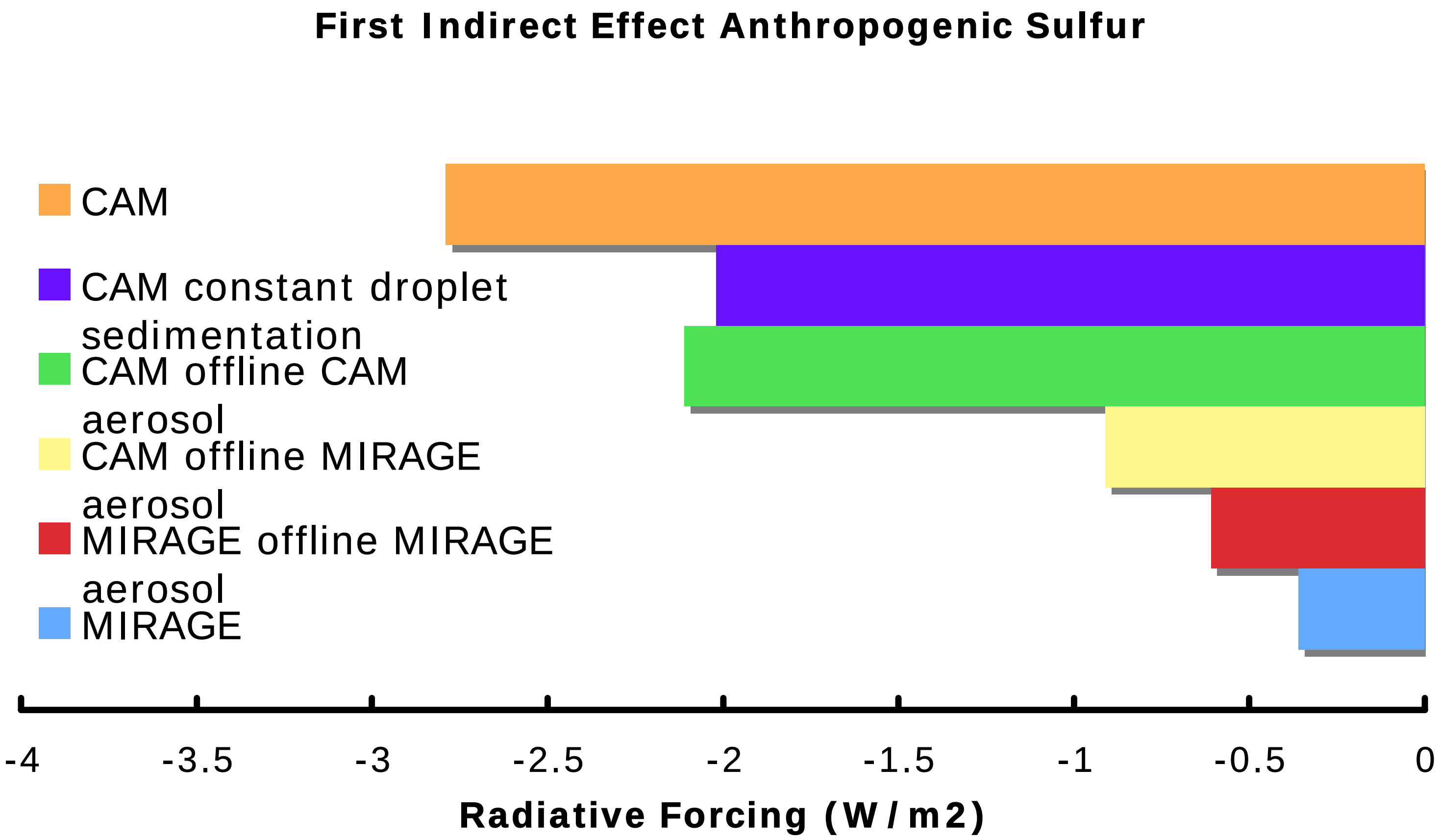
Estimating Direct and Indirect Effects

- **Simulations by CAM3 and MIRAGE**
  - **MIRAGE: PNNL aerosol physics applied to CAM2**
  - **CAM: MOZART/Rasch aerosol applied to CAM3**
  - **Droplet number influences droplet effective radius.**
  - **Dependence of autoconversion on droplet number is neglected**
- **Model Configurations**
  - **4˚ latitude × 5 ˚ longitude × 26 layers**
  - **3-year simulation after 4-month spinup**
- **Estimating Direct and Indirect Effects**
  - **Simulations with, w/out anthropogenic sulfate**
  - **Each simulation calculates radiative fluxes with (F_{aer}) and without any aerosols (F_{noaer}).**
  - **Direct effect of all aerosols in a simulation is $F_{direct} = F_{aer} - F_{noaer}$.**
  - **Difference between simulations is Δ. Then**

$$\begin{aligned} \Delta F_{direct} &= \Delta F_{aer} - \Delta F_{noaer} \\ \Delta F_{indirect} &= \Delta F_{aer} - \Delta F_{direct} \\ &= \Delta F_{noaer} \end{aligned}$$

CAM3 vs. MIRAGE2

First Indirect Effect (courtesy by Steve Ghan, PNNL)



Coupling Air Quality and Meteorology/Climate Modeling

Major Challenges and Future Directions

- Represent climate-aerosol-chemistry-cloud-radiation feedbacks
  - Two-way/chain effects, size-/comp-resolved, multiple sizes, and subgrid variability
  - Real-time emissions, new particle formation, SOA, and aerosol/cloud interaction
- Represent complexity within the computational constraint
  - Development of benchmark model and simulation
  - Characterization of model biases, uncertainties, and sensitivity
  - Develop bias-correction techniques (e.g., chemical data assimilation)
  - Optimization/parameterization of model algorithms with acceptable accuracy
- Develop unified global-through-urban modeling system
  - Globalization/downscaling with consistent model physics
  - Two-way nesting with mass conservation and consistency
- Integrate model evaluation and improvement
  - Laboratory/field studies to improve understanding of major properties/processes
  - Real-time data (e.g., AirNow and Satellite) for data assimilation/model evaluation
  - Development of process-oriented models to isolate complex feedbacks

Coupling Air Quality and Meteorology/Climate Modeling

Ongoing/Near Future Activities

- WRF/Chem
  - NCAR/NOAA/PNNL/NCSU Mesoscale versions
  - BAMS WRF/Chem-SMOKE
  - NCSU global-through-urban WRF/Chem
- CAM3/CAM4
  - NCAR global version with MOZART4 aerosol module
  - PNNL global version with MIRAGE2 aerosol module
  - NCAR downscaling and coupling with WRF/Chem
- Other Online Models
  - EPA: WRF/CMAQ
  - Illinois State Water Survey/UIUC: CWRF/Chem (MOZART4+CMAQ)
  - UC Davis: WRF/PMSO (Source-Oriented PM module)

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