Online Chemistry within WRF: A State-of-the-Art Multi-Scale Air Quality and Weather Prediction Model

Georg Grell

+ many national and international collaborators

WRF/Chem web site - http://wrf-model.org/WG11 http://www.wrf-model.org/WG11

Weather Research and Forecasting (WRF) Model

WORKING GROUP 11: ATMOSPHERIC CHEMISTRY

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Mission

The mission of the atmospheric chemistry working group is to guide the development of the capability to simulate chemistry and aerosols — online as well as offline — within the WRF model. The resulting WRF/Chem model will have the option to simulate the coupling between dynamics, radiation and chemistry. Uses include forecasting chemical-weather, testing air pollution abatement strategies, planning and forecasting for field campaigns, analyzing measurements from field campaigns and the assimilation of satellite and in-situ chemical measurements.

Interaction with other WRF Groups

The initial development of WRF/Chem is involved with the Numerics and Model Dynamics (WG1), Model Physics (WG5), and Land Surface Modeling (WG14).

Community Involvement

2006 WRF workshop working group 11 meeting minutes

Known issues with the WRF model.

Known issues with the WRF/Chem model.

Email WRF/Chem help with question regarding WRF/Chem model.

WRF/Chem related announcements.

Notes from last years mini tutorial on the WEB, a full online tutorial will be released by July 2008

Non-hydrostatic Model Solvers within WRFV2.2 Common Infrastructure

- Eulerian flux-form mass coordinate (Advanced Research WRF, ARW core)
- NMM model (Non-hydrostatic Mesoscale Model, NCEP's core)

Many different physics options (MM5-ETA-RUC….), now for both cores!!

Also available: 3DVAR systems (WRF, GSI) for meteorological analysis, FDDA nudging for ARW

WRF/Chem

Community effort

Largest contributing groups: ESRL, PNNL, NCAR

Other significant contributions from: MPI Mainz, CPTEC Brazil, CDAC India, U of Chile

WRF/chem

- Online, completely embedded within WRF CI
- Consistent: all transport done by meteorological model
  - Same vertical and horizontal coordinates (no horizontal and vertical interpolation)
  - Same physics parameterization for subgrid scale transport
  - No interpolation in time
- Easy handling (Data management)
- Modular approach
  - Chemistry subdirectory has been implemented in versions of HIRLAM and RAMS

Deposition/Biogenic Emissions

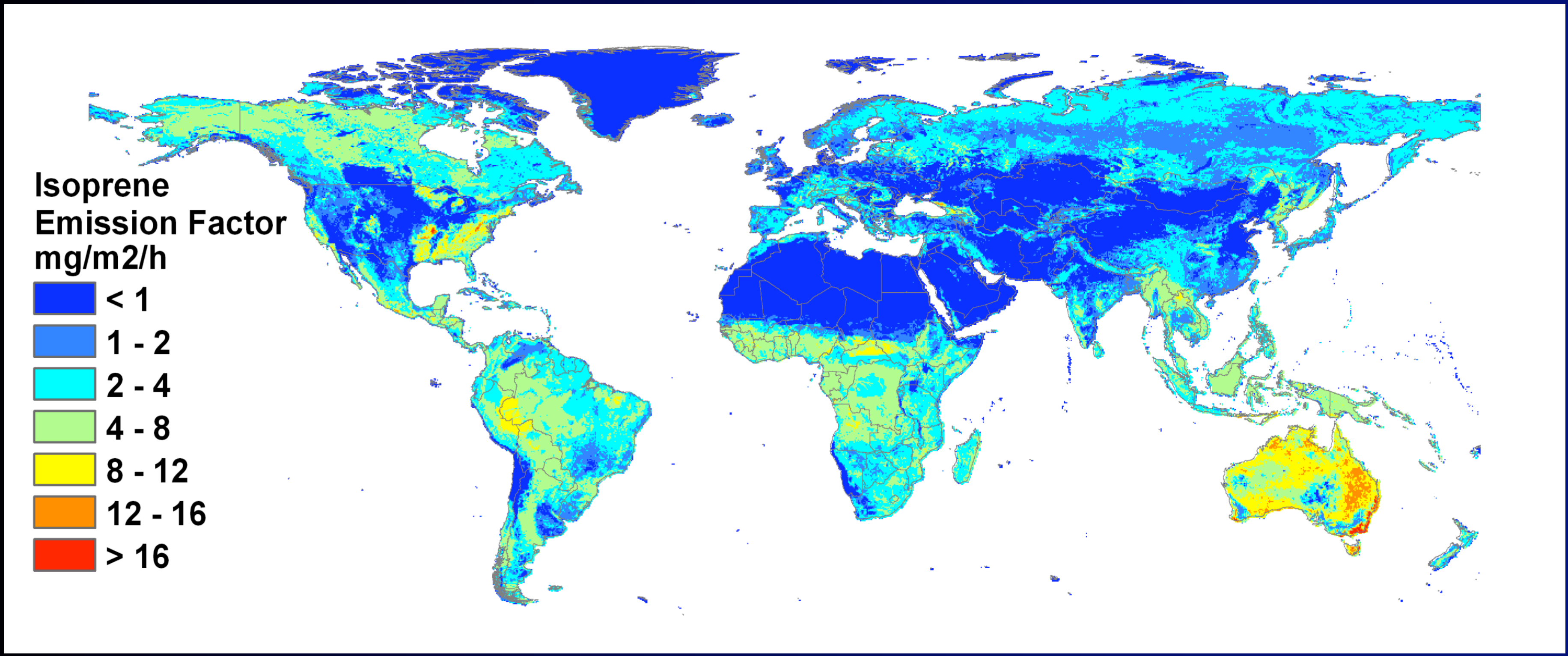
- Dry deposition (coupled with soil/veg scheme, "flux-resistance" analogy)
- Simplified wet deposition by convective parameterization (scavenging factor of .6 for aerosols, no aqueous-phase chemistry involved)
- Biogenic emissions (as in Simpson et al. 1995 and Guenther et al. 1994), include temperature and radiation dependent emissions of isoprene, monoterpenes, also nitrogen emissions by soil
  - May be calculated "online" based on USGS landuse
  - May be input
  - BEISv3.13(offline reference fields, online modified)

Implementation of the ***M***odel of ***E***missions of ***G***ases and ***A***erosols from ***N***ature MEGAN in WRFV2-Chem (Courtesy of Christine Wiedinmyer and Alex Gunther from NCAR, also Serena Chung, and Jerome Fast)

Code is available will officially be released with V3 in March of 2008

MEGAN: Model of Emissions of Gases and Aerosols from Nature

- Global biogenic emissions model
  - 1 km^2 spatial resolution
  - Predicts emissions of > 50 VOC



Gas Phase Chemistry Packages

- Chemical mechanism from RADM2 (Quasi Steady State Approximation method with 22 diagnosed, 3 constant, and 38 predicted species is used for the numerical solution)
- Carbon Bond (CBM-Z) based chemical mechanism, and the
- ***K***inetic ***P***re***P***rocessor (KPP)

KPP: Kinetic PreProcessor (Damian et al, 2002, Sandu et al, 2003, Sandu and Sander 2006)

- **Automatic tool to generate chemical mechanisms with a choice of time integration schemes**
- **Can also generate adjoints**
- **Well documented, tested, and widely used**

Thanks go to Marc Salzman from the MPI in Mainz

Current gas-phase mechanism equation files for KPP that are used in WRF/Chem:

- RADM2
- RACM
- RACM-MIM
- RACM-jpl
- Mainz MPI global mechanism
- CB4 (to be released for V3)

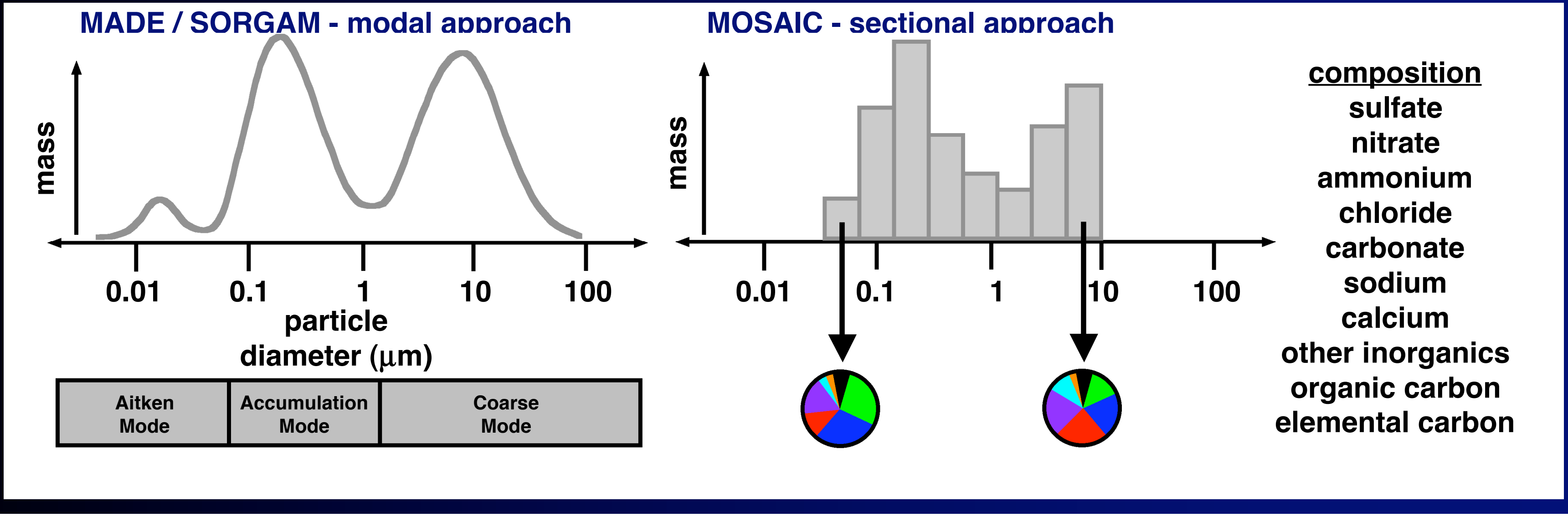
Available Aerosols modules

1. PM advection, transport, emissions and deposition only
2. Modal approach (MADE/SORGAM)
3. Sectional approach (MOSAIC)

Aerosol direct and indirect effect has been implemented by PNNL for the Goddard radiation scheme and the Lin et al. microphysics

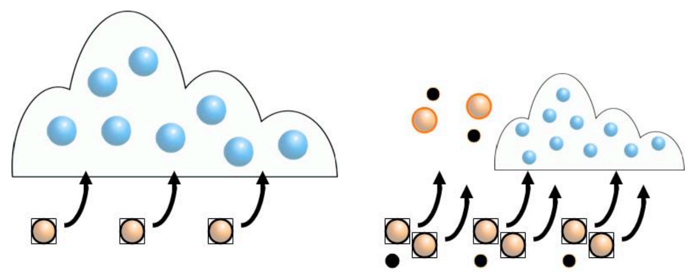
MOSAIC

- Sectional size distribution; moving-center or two-moment approach for the dynamic equations for mass and number; 112 prognostic species
- Mixing rule for activity coefficients of various electrolytes in multi-component aqueous solutions [*Zaveri et al., JGR, 2005*]
- Thermodynamic equilibrium solver for solid, liquid, or mixed phase state of aerosols [*Zaveri et al., In Press JGR, 2006*]
- Dynamic integration of the coupled gas-aerosol partitioning differential equations [*Zaveri et al., In preparation*]



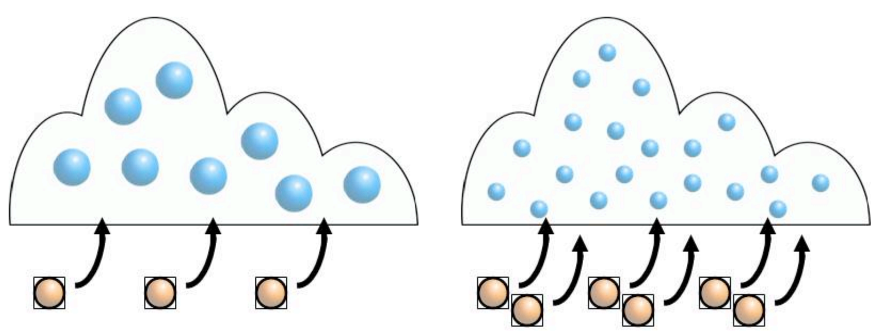
Aerosol effects included in WRF/Chem

Semi-Direct Effect



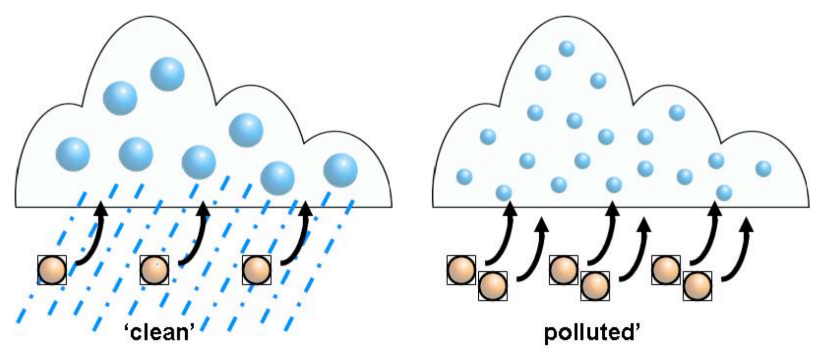
- Influence of aerosol absorption of sunlight on formation and evaporation of clouds

First Indirect Effect



- Influence of cloud optical depth through impact on effective radius, with no change in water content of cloud

Second Indirect Effect



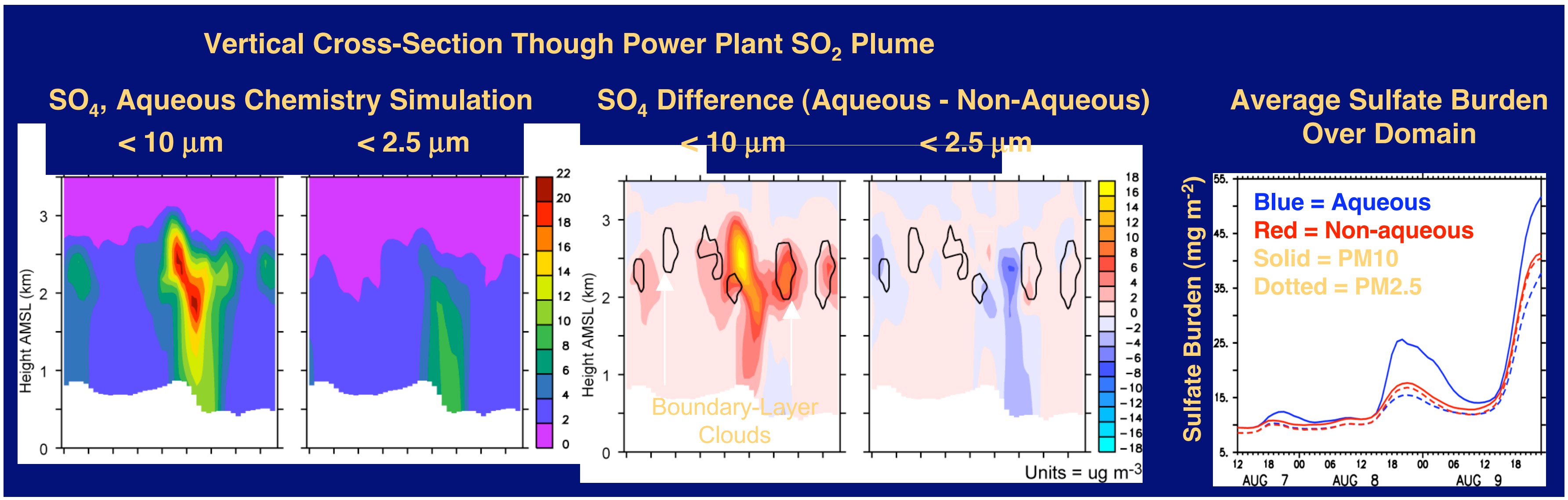
- Influence of cloud optical depth through influence of droplet number on mean droplet size and hence initiation of precipitation

Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy

Cloud-Aerosol Interactions

Aqueous Chemistry

- Bulk cloud-chemistry module of *Fahey and Pandis* [2001]
- Oxidation of S(IV) by H_2O_2, O_3, trace metals, and radical species
- Non-reactive uptake of HNO_3, HCl, NH_3, and other trace gases
- Bulk mass changes partitioned among cloud-borne aerosol size bins, followed by transfer of mass & number between bins due to growth



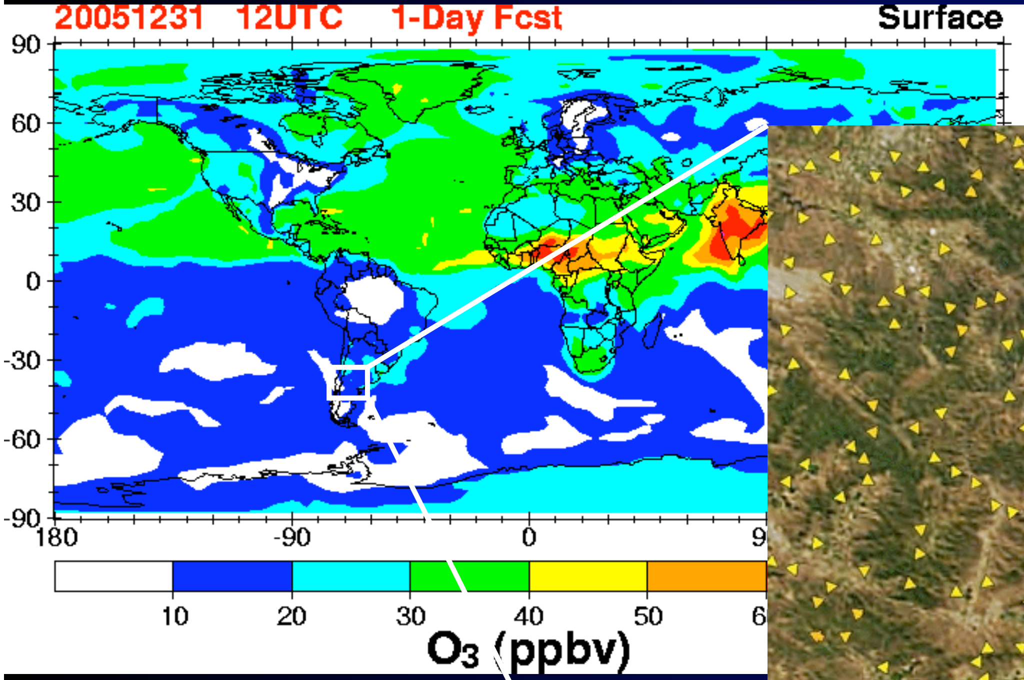
Aerosol Interactions Not Treated Yet

- **First Dispersion Effect:** Influence on cloud optical depth through influence of aerosol on dispersion of droplet size distribution, with no change in water content of cloud
- **Second Dispersion Effect:** Influence on cloud optical depth through influence of aerosol on dispersion and hence initiation of precipitation
- **Glaciation Indirect Effect:** Influence of aerosol on conversion of haze and droplets to ice crystals, and hence on cloud optical depth and initiation of precipitation

Photolysis Packages – all coupled to aerosols and hydrometeors

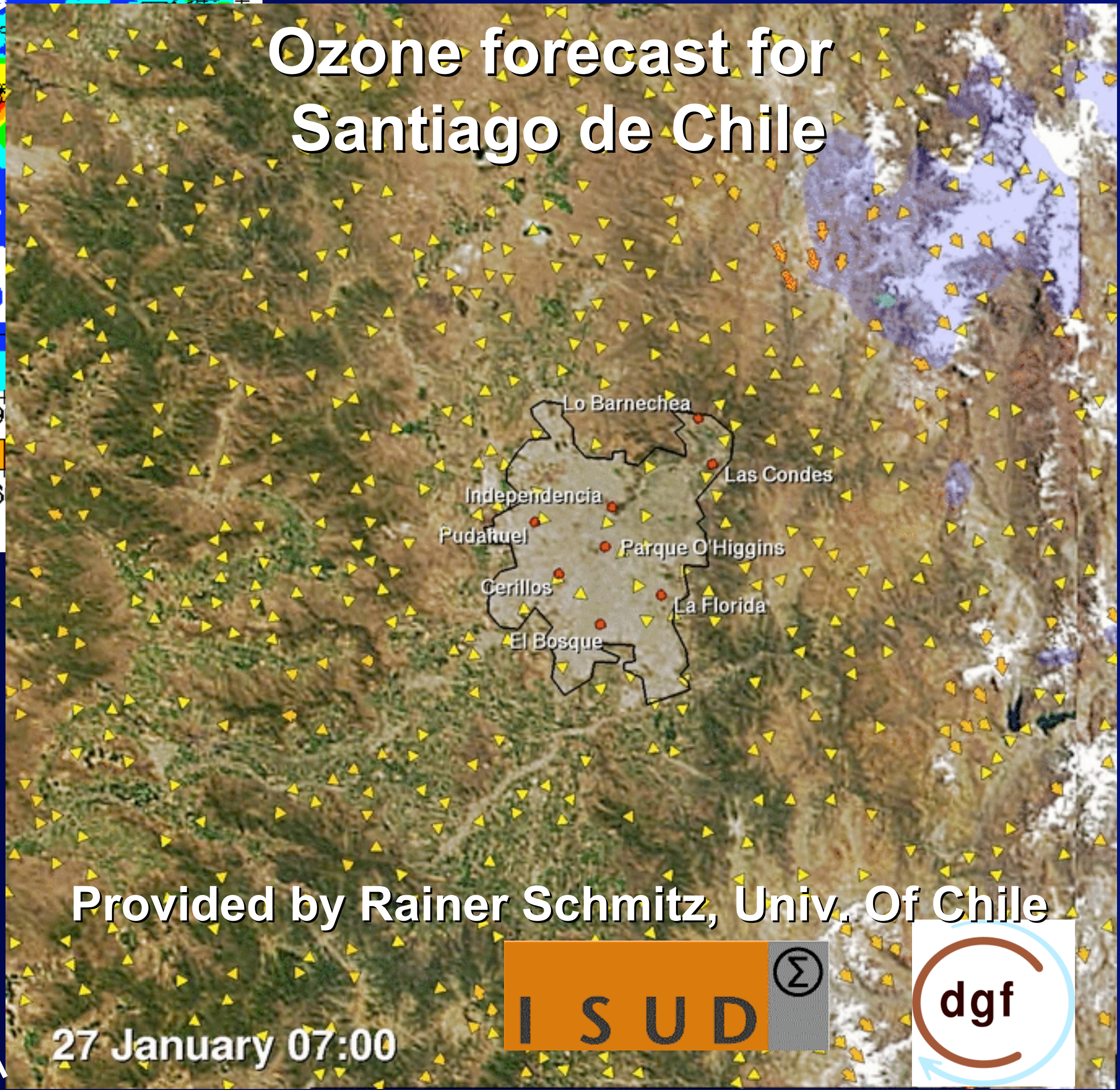
- Fast-j photolysis scheme
- Madronich Photolysis
- Madronich FTUV code available , official release with V3)

Use of chemical data from Global Chemistry Model (GCM) for boundary conditions, or 1-way nest, or 2-way nest



Global forecast by Max-Planck-Instiute, Mainz, Germany (Lawrence, 2003)

<u>Now also available for MOZART and RAQMS and of course WRF/Chem</u>



Improved non-resolved convective transport

- Ensemble approach (based on Grell/Devenyi parameterization)
  - Uses observed or predicted rainfall rates as met-input
  - Ensemble of entrainment/detrainment profiles and/or downdraft parameters to determine vertical redistribution of tracers
  - Ensembles may be weighted to determine optimal solution
  - Can be used as 3-d scheme for smooth transition to high resolution
- Aqueous phase chemistry module called from within convective routine, CMAQ module (not tested and released yet)
- Connected to photolysis and atmospheric radiation schemes

A model within a model : Fire Plumerise (Collaboration with Saulo Freitas from CPTEC in Brazil)

Initialized with GOES-ABBA and MODIS

1-D Plume model

$$\frac{\partial w}{\partial t} + w\frac{\partial w}{\partial z} = \gamma g B - \frac{2\alpha}{R} w^2 \quad \begin{cases} \gamma = \frac{1}{1+0.5} & \text{[illegible]} \\ \gamma = \frac{1}{1-2\mu} & \text{[illegible]} \end{cases}$$

$$\frac{\partial T}{\partial t} + w\frac{\partial T}{\partial z} = -w\frac{g}{c_p} - \frac{2\alpha}{R}|w|(T - T_e) + \left(\frac{\partial T}{\partial t}\right)_{microphysics}$$

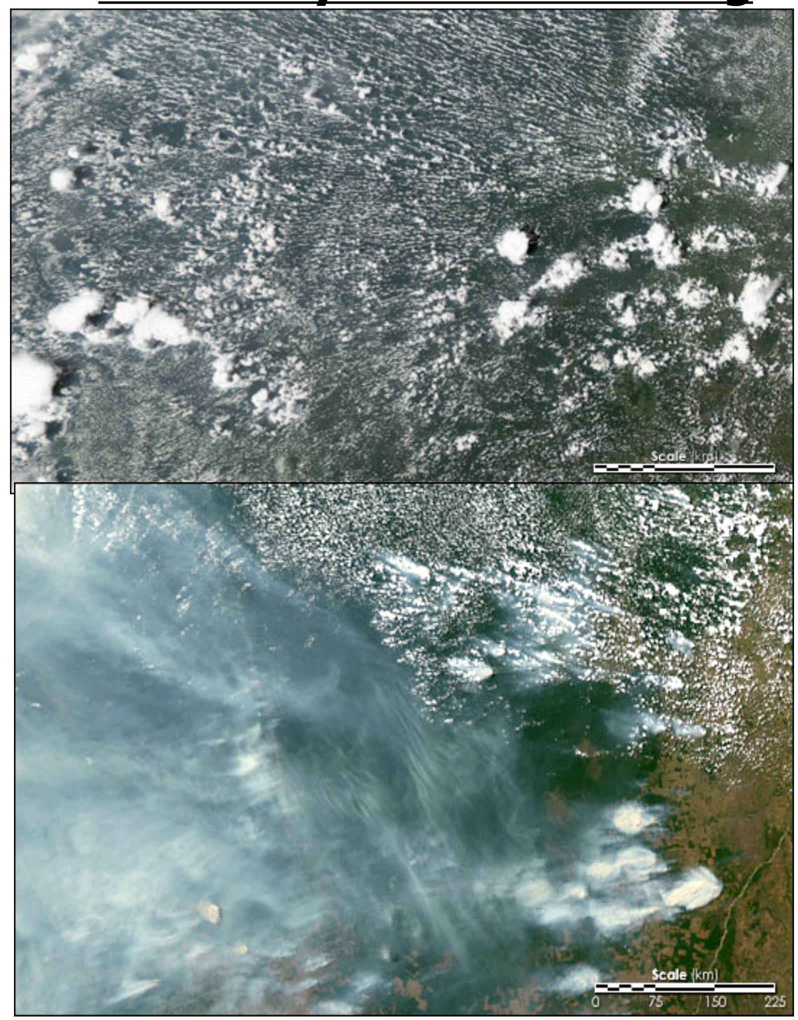
$$\frac{\partial r_v}{\partial t} + w\frac{\partial r_v}{\partial z} = -\frac{2\alpha}{R}|w|(r_v - r_{v,e}) + \left(\frac{\partial r_v}{\partial t}\right)_{microphysics}$$

$$\frac{\partial r_c}{\partial t} + w\frac{\partial r_c}{\partial z} = -\frac{2\alpha}{R}|w| r_c + \left(\frac{\partial r_c}{\partial t}\right)_{microphysics}$$

$$\frac{\partial r_{ice,rain}}{\partial t} + w\frac{\partial r_{ice,rain}}{\partial z} = -\frac{2\alpha}{R}|w| r_{ice,rain} + \left(\frac{\partial r_{ice,rain}}{\partial t}\right)_{microphysics} + sedim$$

$$\left(\frac{\partial \xi}{\partial t}\right)_{microphysics} (\xi = T, r_v, r_c, r_{rain}, r_{ice}), \quad sedim \begin{cases} \text{bulk microphysics:} \\ \text{Kessler, 1969} \\ \text{Ogura \& Takahashi, 1971} \\ \text{Berry, 1967} \end{cases}$$

Semi-direct (?) effect caused by biomass burning

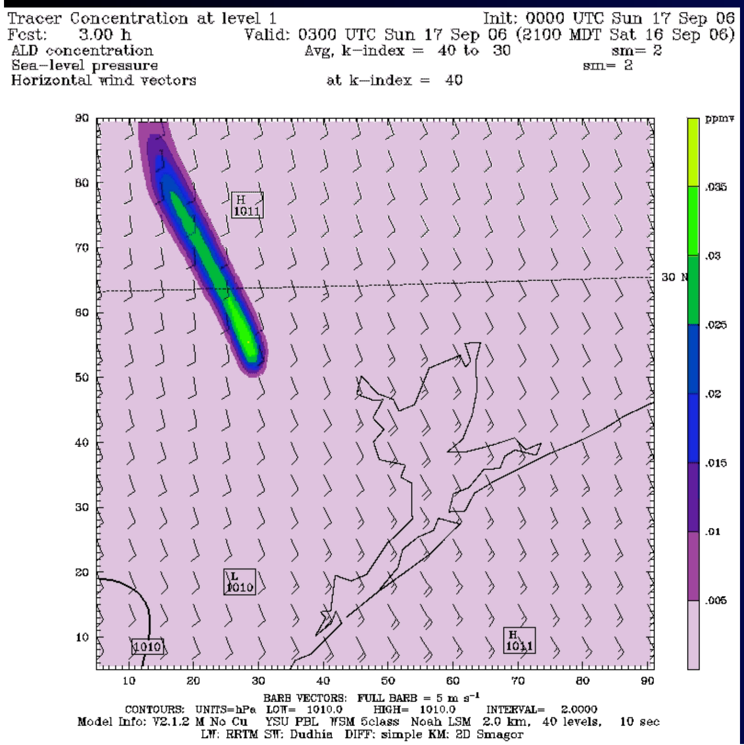


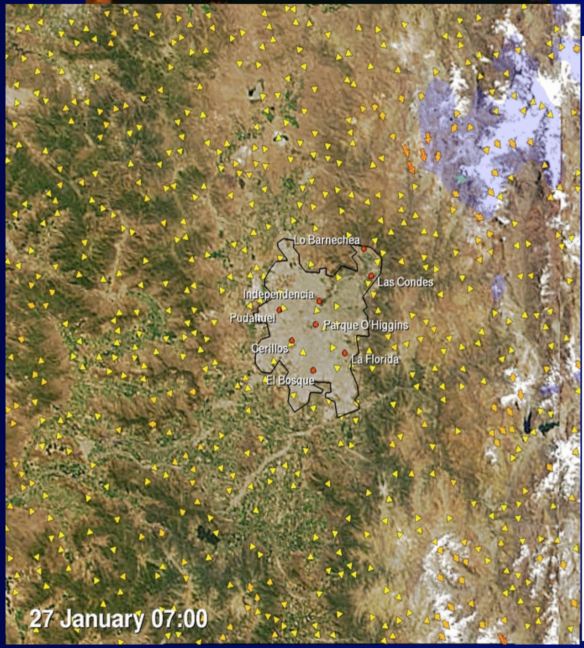
Near future (for release V3 in March)

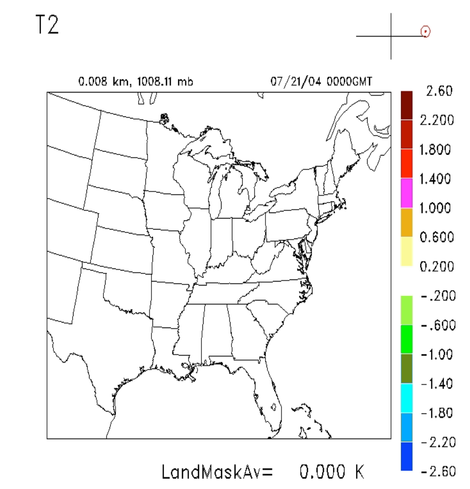
- Global WRF/Chem
  - KPP equation file for global gas-phase mechanism from MPI Mainz
  - RETRO or EDGAR emissions data set
  - Global fire emissions from GOES-ABBA and MODIS
- Sea Salt parameterization (courtesy of M. Sofiev)
- Coupling of modal aerosol approach with radiation schemes (J. Fast)
- Possibly GOCART Sea Salt and Dust modules

Current possible applications

AQ/weather/climate linkage







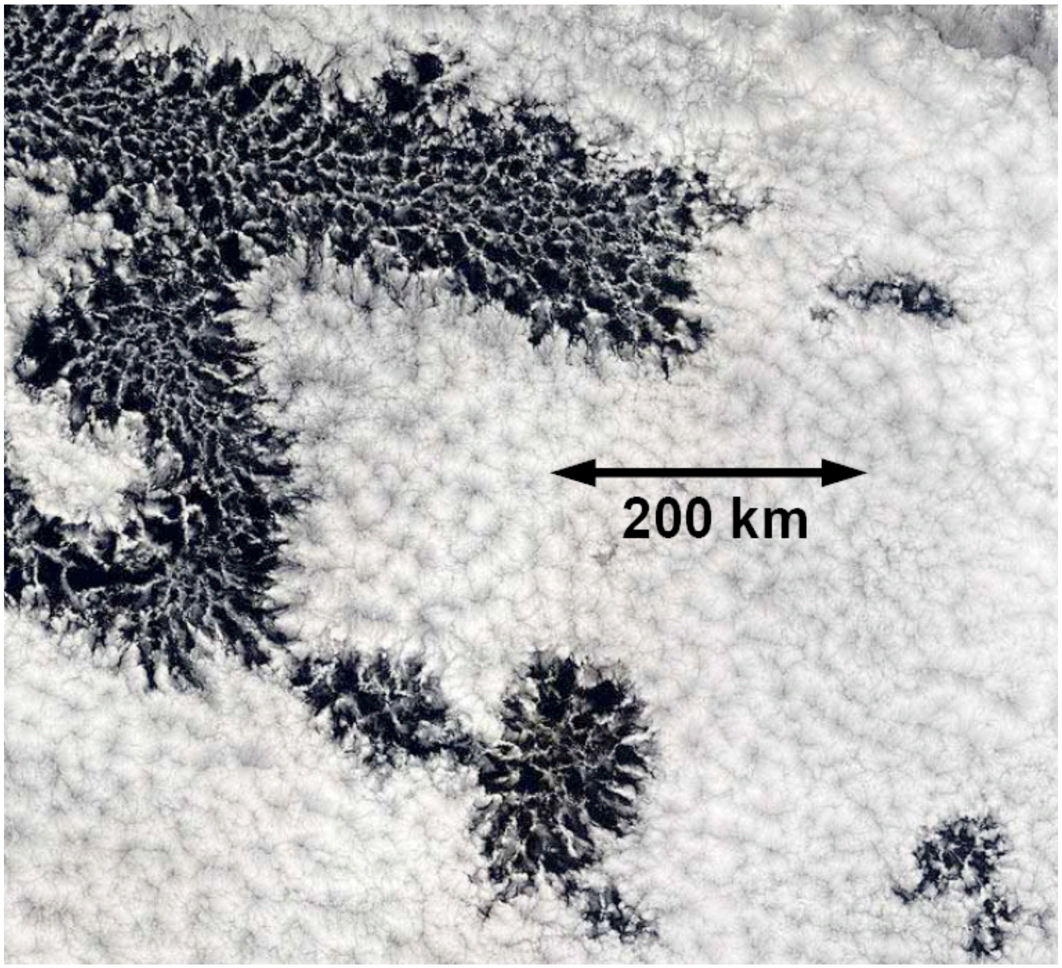
Distant line-up for WRF/Chem, with various groups working on these issues

- More aerosol modules
- Chemical data assimilation
  - 4dvar work in collaboration with Greg Carmichael and Dale Barker using WRF-var
  - 3dvar work at ESRL using GSI
- More choices for “interactive” parameterizations
  - CAMS radiation package
  - Various microphysics packages
  - GD convection parameterization

WRF/Chem Aerosol related work

- Graham Feingold and Hailong Wang (ESRL/CSD): Implementation of TelAviv sectional microphysics that includes CCN activation, condensation/evaporation, stochastic collection, and sedimentation
- Graham Feingold and Hailong Wang (ESRL/CSD): Implementation of double moment bulk microphysics scheme (Feingold et al. 1998)
- Gordon McFiggans (U of Manchester, UK), implementing their multicomponent aerosol approach
- Laura Fowler and others from CSU, implementing some of the RAMS microphysics routines into WRF
- Karla Longo and Saulo Freitas (CPTEC, Brazil) looking at aerosol direct effect with BRAMS and WRF/Chem

Model aerosol effects on the formation and evolution of POCs and on precipitation in POCs examine factors that control macrophysical and microphysical properties of Sc



- Satellite imagery shows the recurrence of Pockets of Open Cells (POCs) in otherwise unbroken marine stratocumulus (Sc).
- POCs regions have smaller cloud cover and are optically thinner than unbroken Sc fields.
- POCs are often associated with enhanced precipitation, which may susceptible to aerosol loading (the second aerosol indirect effect).
- Evaporative cooling from precipitation in POCs may produce “cool pools” that affect mesoscale organizations.

Warm-rain microphysics

- Explicit bin-resolving microphysics (roughly 35 bins, TelAviv microphysics)
  - CCN activation, condensation/evaporation, stochastic collection, and sedimentation
- Double-moment bulk microphysics (Feingold et al. 1998)
  - Mass and number concentration of cloud droplets and rain drops are predicted;
  - Log-normal distributions;
  - Activation is based on equilibrium theory;
  - Condensation/evaporation is computed using analytical method, no saturation adjustment is assumed;
  - Lookup tables generated from bin microphysics for collection and sedimentation.

Applications of the WRF/Chem model within ESRL/CSD

Stu McKeen, Si-Wan Kim, Greg Frost, Serena Chung (ESRL/CSD and CU/CIRES)

Evaluation: WRF/Chem in weather/air-quality forecast mode

- Evaluations using data from ICARTT/NEAQS-2004
  - Surface Network for O_3 and $PM_{2.5}$
  - Ronald H Brown Ship data in the Gulf of Maine
  - NOAA WP-3 aircraft measurements - detailed chemistry
  - NOAA DC-3 Ozone lidar measurements
- Evaluations using data from TexaQS06

WRF/Chem as a research tool – important also for global change applications

- Changes in Anthropogenic Emissions - Satellite comparisons
- Aerosol-Radiation-Meteorology Interactions
- Testing of PBL parameterizations

Model variables available for Comparison with NOAA Aircraft and Ron Brown data

gas phase chemistry

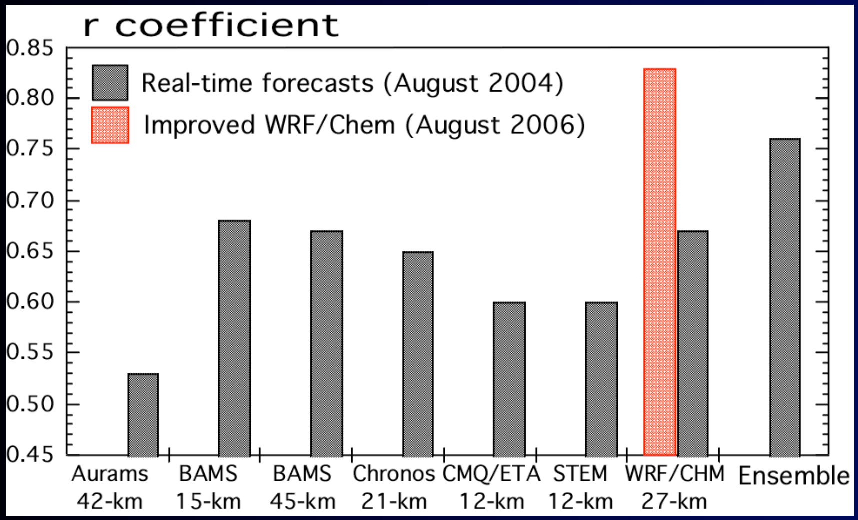
	AURAMS	CHRONOS	STEM	WRF-2
O_3	√	√	√	√
CO			√	√
NO	√	√	√	√
NOx	√	√	√	√
NOy	√	√	√	√
PAN	√	√	√	√
Isoprene	√	√	√	√
SO_2	√	√	√	√
NO_3	√	√		√
N_2O_5	√	√		√
CH_3CHO	√			√
Toluene		√		√
Ethylene	√	√		√
NH_3				√

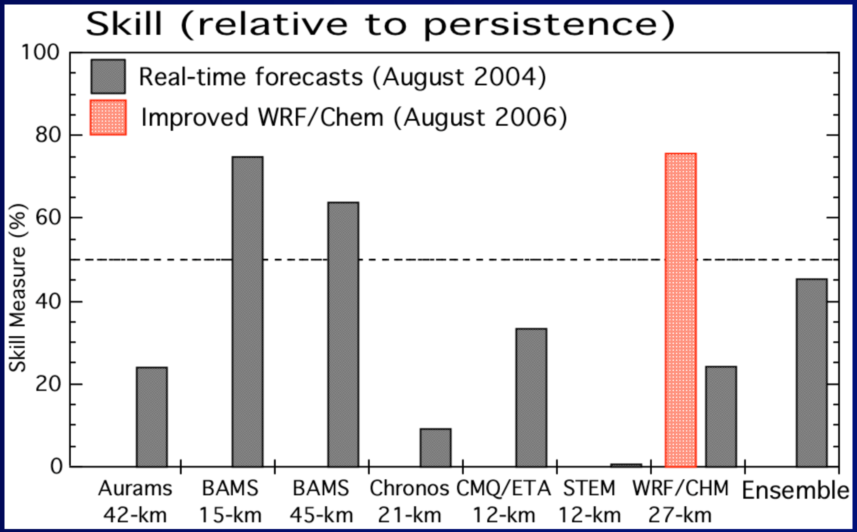
aerosols, radiation, meteorology

	AURAMS	CHRONOS	STEM	WRF-2
PM2.5	√	√	√	√
Asol SO_4	√	√	√	√
Asol NH_4	√			√
Asol OC	√	√	√	√
Asol EC	√		√	√
Asol NO_3	√			√
JNO_2				√
T	√	√	√	√
P	√		√	√
H_2O	√	√	√	√
winds	√	√	√	√
SST	√			√
Radiation				√

http://www.al.noaa.gov/ICARTT/modeleval/

Improvements in WRF and WRF/Chem from 2004 to 2006: comparisons with AIRNow surface O_3 data



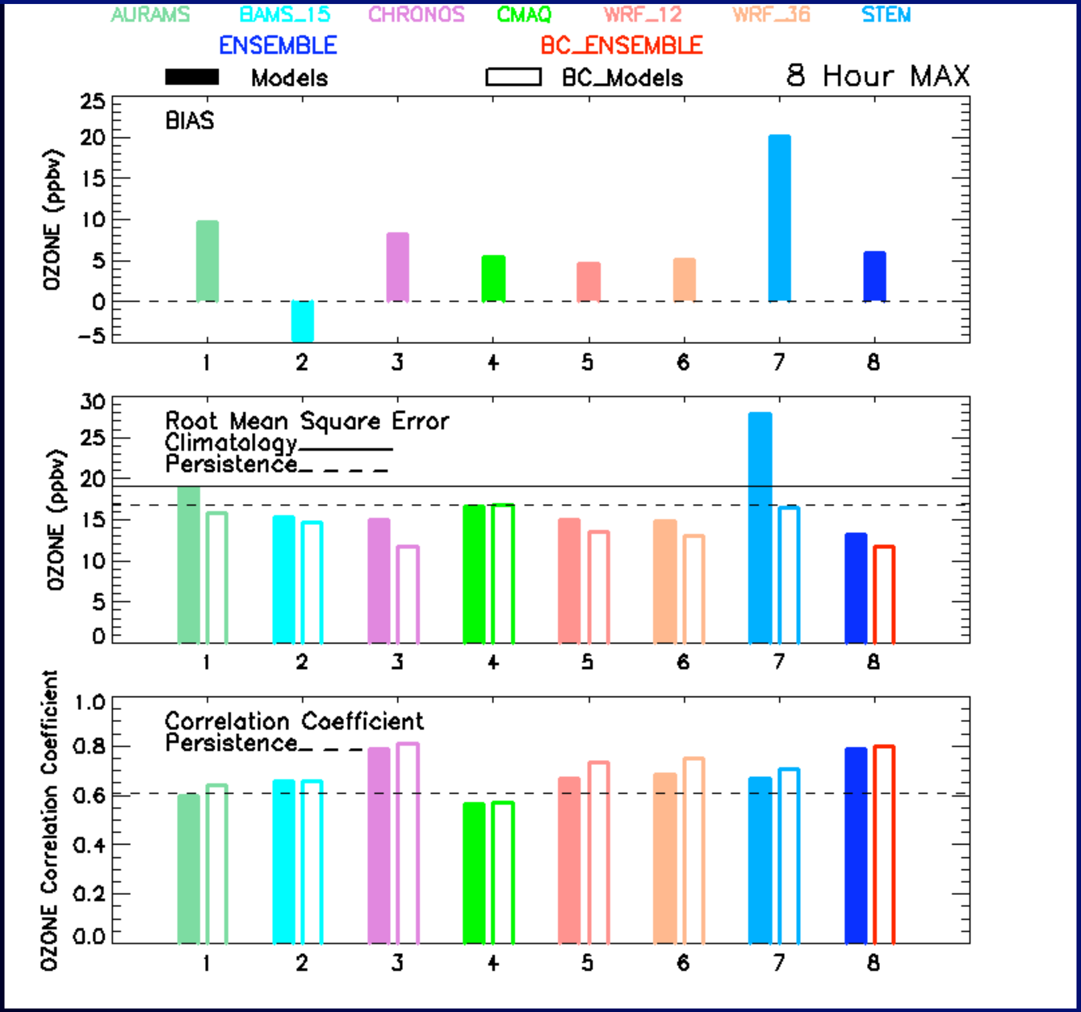


Maximum 8 hour averages

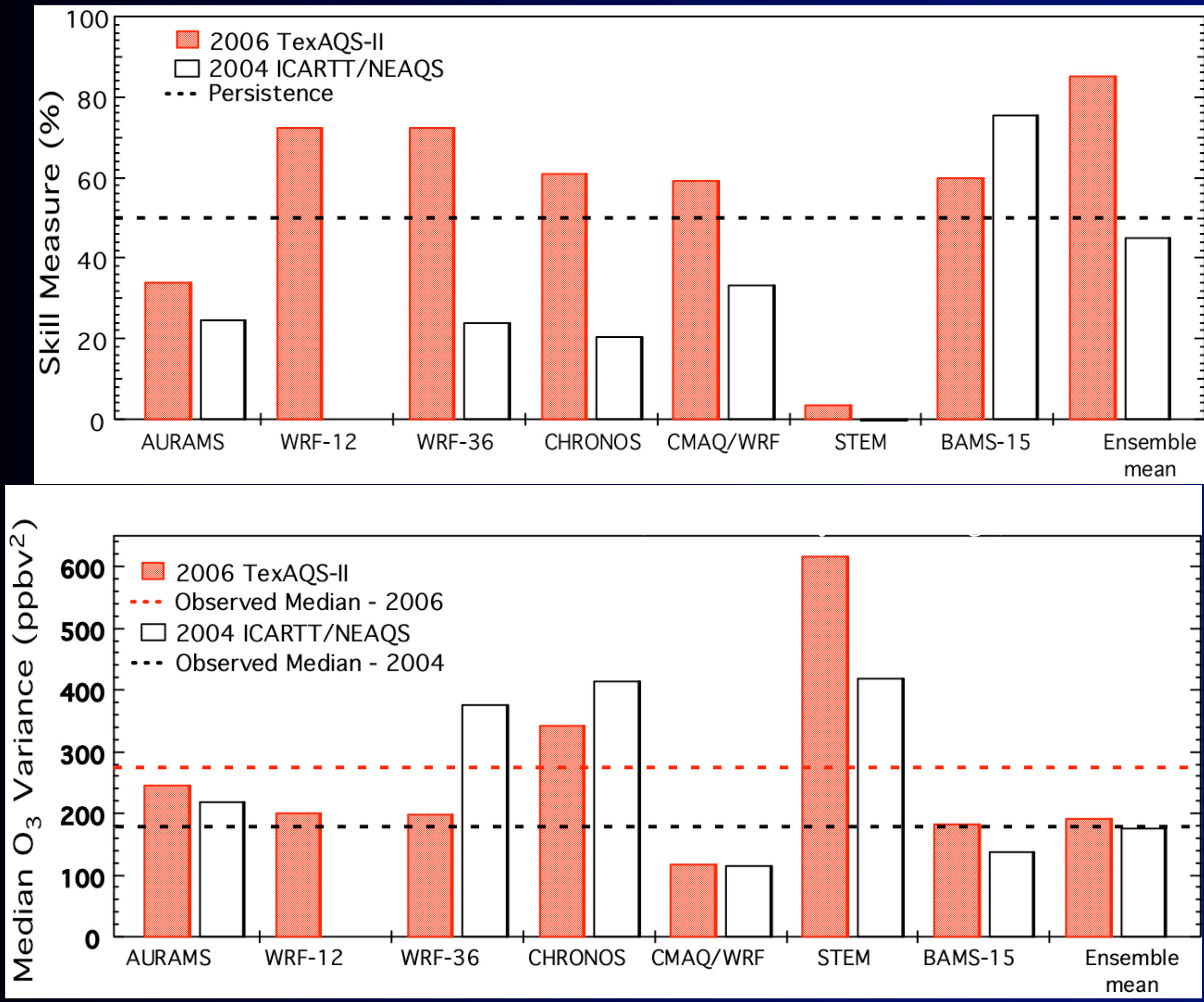
352 O_3 monitors - eastern U.S. and Canada

53 days (July and August 2004)

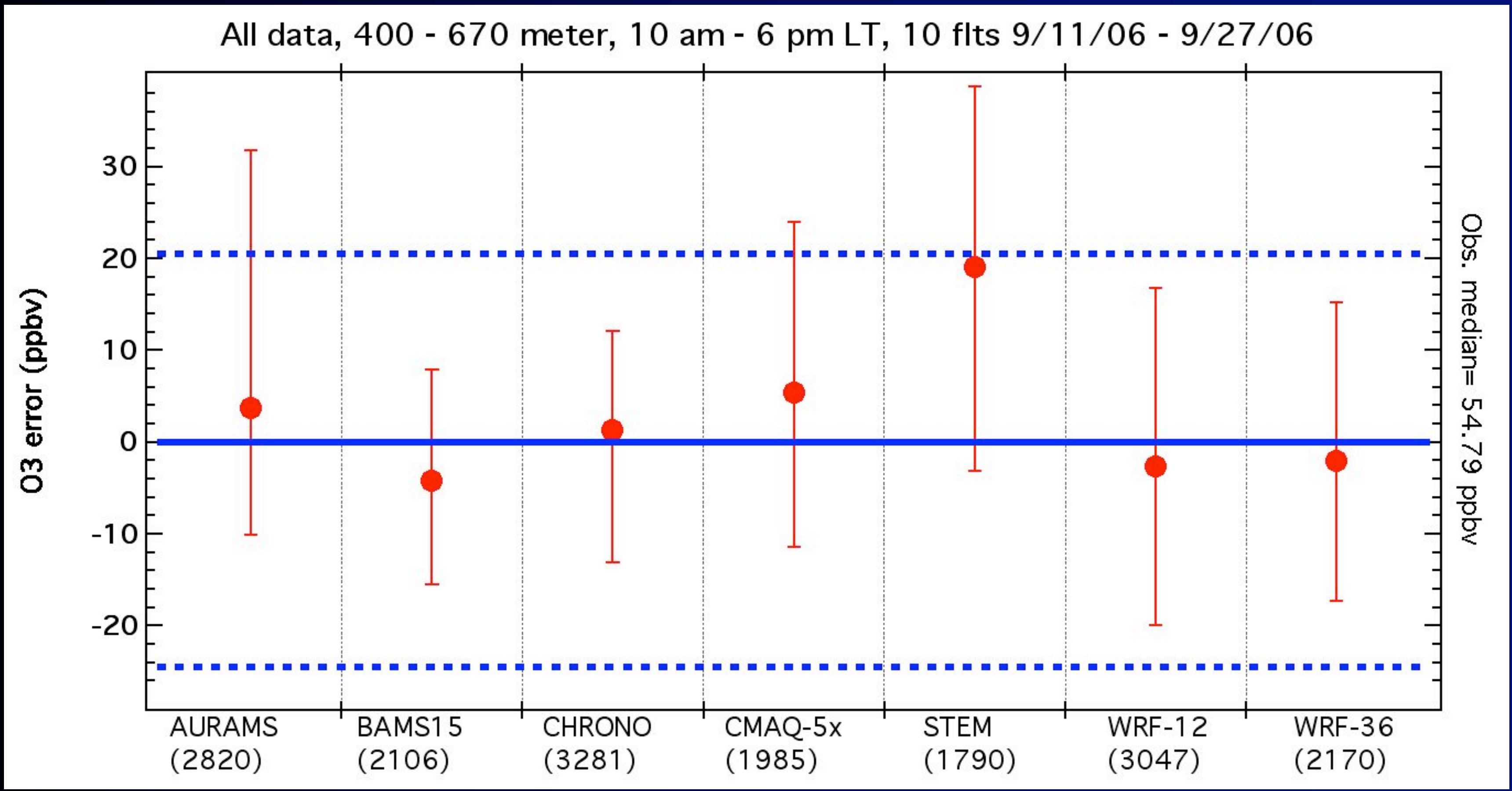
Maximum 8-hr average O_3 statistics for 119 AIRNow monitors in East Texas 8/12/06 - 9/30/06 (Jim Wilczak and Irina Djalalova, NOAA/ESRL/PSD)



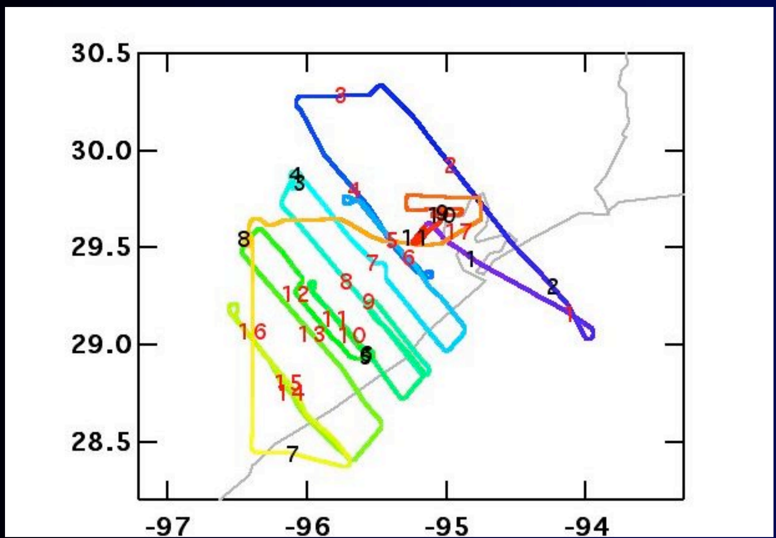
2006 versus 2004 surface O_3 statistics (no bias corrections)

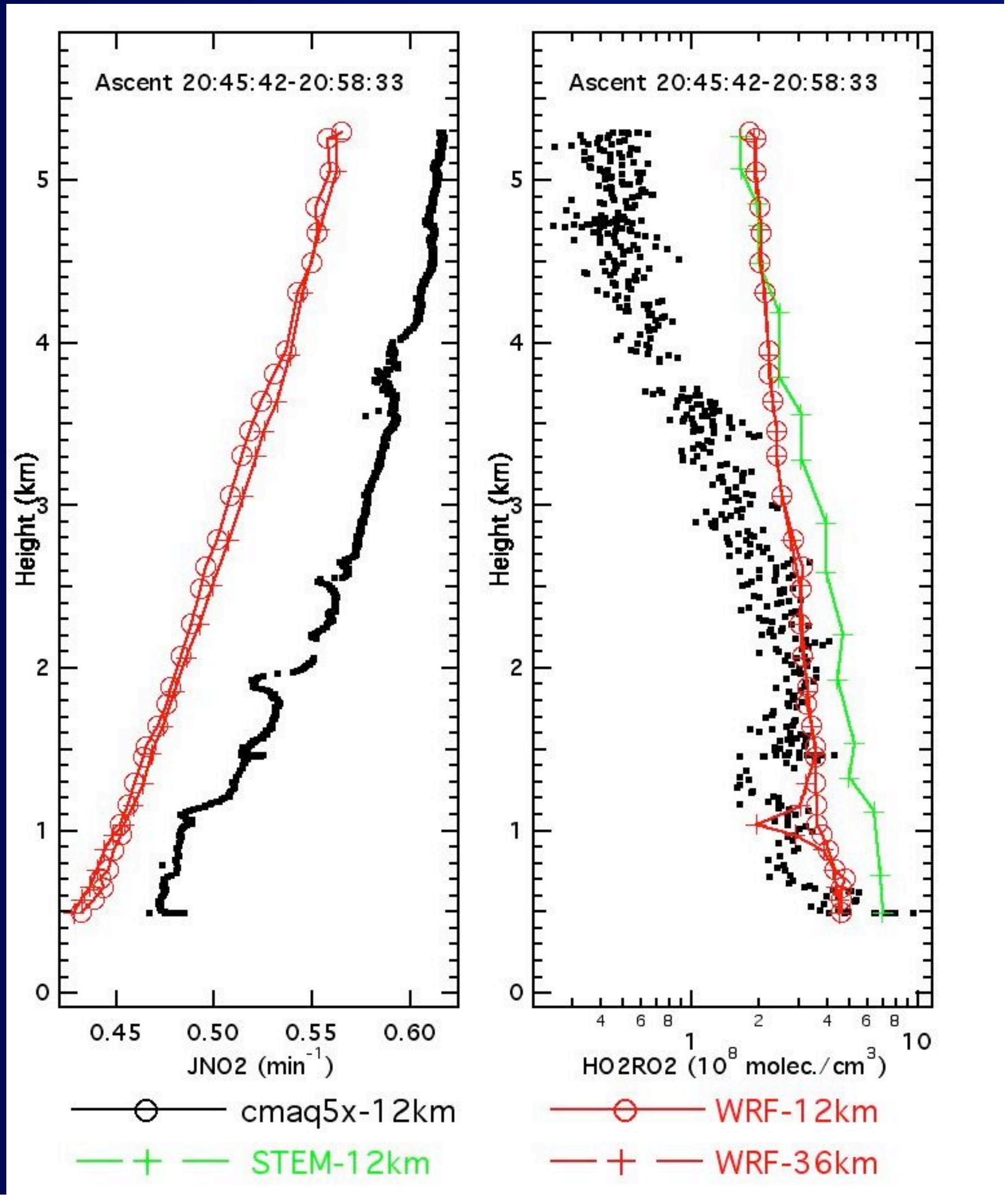


Model to model bias comparisons for O_3 in the mid-day PBL

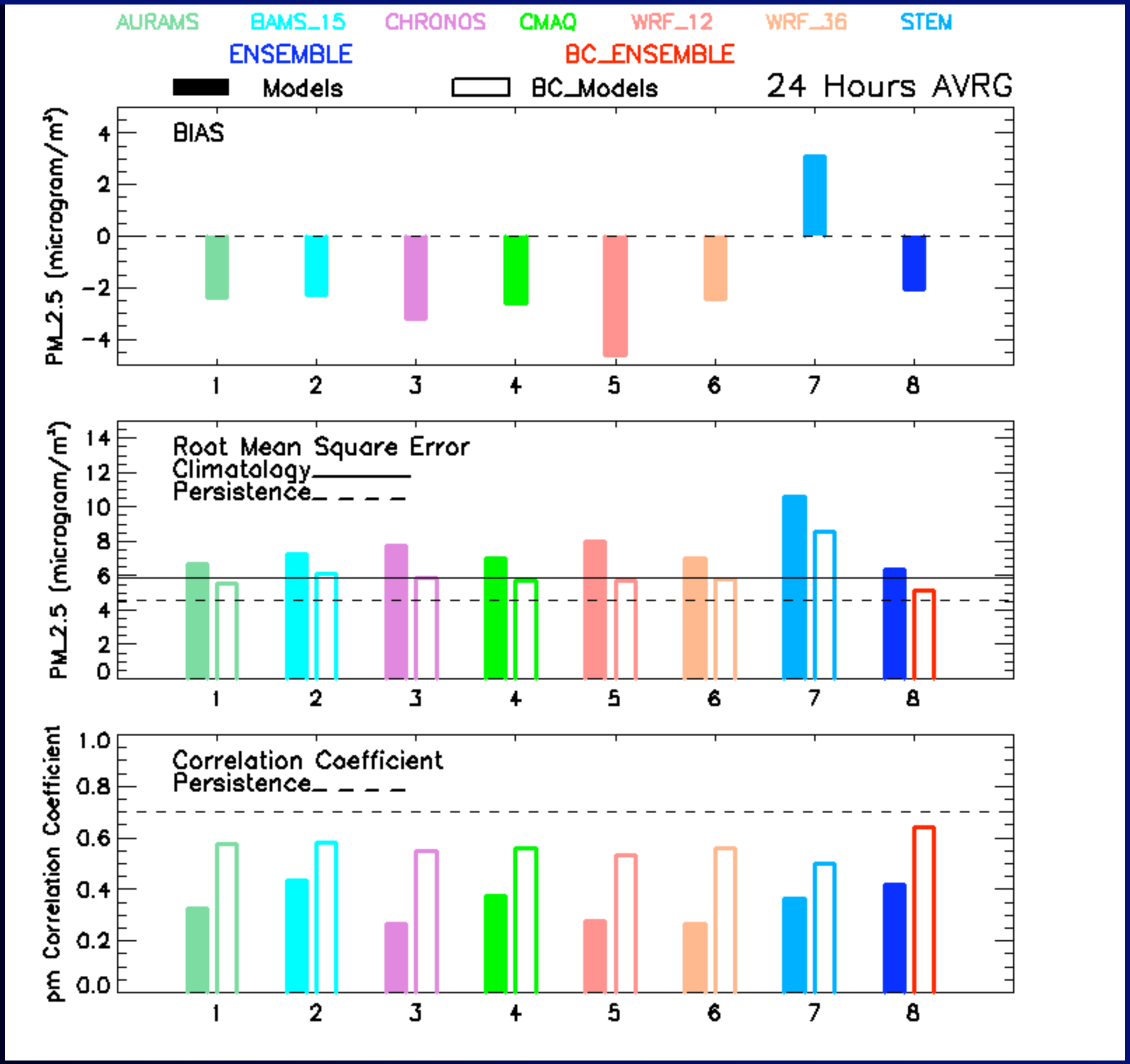


Texas 2006 – aircraft comparisons





24-hr average $PM_{2.5}$ statistics for 38 AIRNow monitors in East Texas 8/13/06 - 9/30/06 (Jim Wilczak and Irina Djalalova, NOAA/ESRL/PSD)



Resources

- WRF project home page
  - http://www.wrf-model.org
- WRF users page (linked from above)
  - http://www.mmm.ucar.edu/wrf/users
- On line documentation (also from above)
  - http://www.mmm.ucar.edu/wrf/WG2/software_v2
- WRF users help desk
  - wrfhelp@ucar.edu
- WRF/Chem users help desk
  - wrfchemhelp.gsd@noaa.gov