Online Chemistry within WRF: Description and Application of a State-of-the-Art Fully Coupled Multi-Scale Air Quality and Weather Prediction Model

Georg Grell

+ many national and international collaborators

Major slide contributors: Jerome Fast, Serena Chung, Stu McKeen, Greg Frost, Marc Salzman, Rainer Schmitz

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

Earth System Research Laboratory
SCIENCE, SERVICE & STEWARDSHIP

Structure of talk

- What was WRF and WRFV2.1/Chem
- New additions in WRFV2.2 (just released)
- Research applications
- Future developments

http://www.wrf-model.org/WG11

WORKING GROUP 11: ATMOSPHERIC CHEMISTRY

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Rainer Schmitz, *IMK-IFU and University of Chile*
Doug Westphal, *USN Research Lab*
Pai-Yei Whung, *NOAA*
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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 (WG11), and Land Surface Modeling (WG14).

Current Status of WRF-chem
Anthropogenic Emissions Available for WRF-chem
Model Evaluation
Future Plans
WRF/Chem FAQs
Real-time Air Quality Forecasts using WRF-chem

This page originally developed by Bill Moninger and Randy Collander and later by Steven Peckham
Model questions should be directed to Georg Grell and Steven Peckham.
Last modified: Monday February 7, 2005 07:00 AM

Directly involved in major WRF/CHEM development – for the current release version

at NOAA/ESRL: **Steven Peckham (NOAA/ESRL/GSD), and Stu McKeen (NOAA/ESRL/CSD), also assists from Serena Chung, Greg Frost, Si Wan Kim**

Major developers in **US**: Jerome Fast, Bill Gustafson (**PNNL**), Bill Skamarock (NCAR)

South America: Rainer Schmitz (U. of Chile)

Europe: Marc Salzmann (MPI Mainz)

India: C-DAC

And other contributions from: **Saulo Freitas (CPTEC Brazil)**, and

Many more national and international collaborators

A few things about the meteorological side of WRF/Chem

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

“Basic” WRF 3DVAR (NCAR, ARW): Observations

Many conventional (surface , upper air) data sources as well as remotely sensed retrieval data

4DVAR in preparation, also collaboration with WG11 on chemical 4DVAR

Contact Dale Barker for questions about WRF-Var (also check WRF-Var WEB-Page

Gridpoint Statistical Interpolation or GSI

- main developer: NCEP/EMC, global *and* regional applications

- operational in NCEP's NMM-WRF since June 2006,

- main partners: NASA/GMAO, ESRL/GSD,

- observation used besides conventional ones come from satellites (AIRS, HIRS, AMSU-A, AMSU-B, GOES Imager, SSM/I, etc.), radar (radial wind), lidar, GPS (ground based and satellite), etc.,

Details are available from

http://www.emc.ncep.noaa.gov/gmb/treadon/gsi/

GSI was used for met-fields in WRF/Chem, may be used in future applications for chemical species

WRF/chem

- As of now: “Online”, sometimes also called “inline”
- Completely embedded within WRF CI
- Consistent: all transport done by meteorology 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)

Chemistry Package – V2.1

- 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
- Fast-j photolysis scheme (coupled to aerosols and microphysics)
- Madronich Photolysis, coupled with hydrometeors and aerosols

Aerosols – V2.1

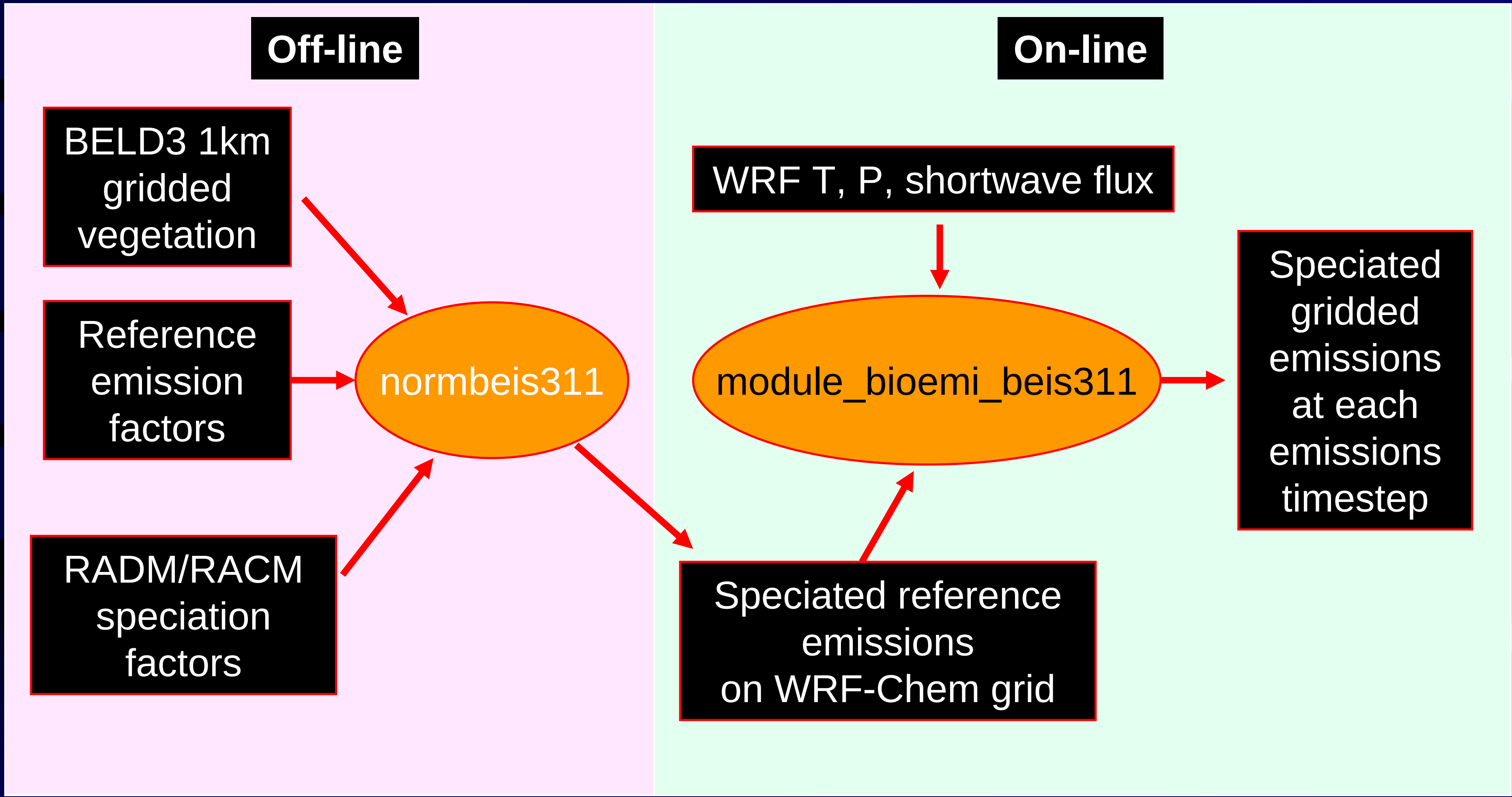
- Based on Modal Aerosol Dynamics Model for Europe (MADE, Ackermann et al. 1998)
- Modified to include Secondary Organic Aerosols (SOA), (Schell et al. 2001)
- Extra transport: total number of aerosol particles within each mode as well as all primary and secondary species for Aitken as well as Accumulation mode
- Diagnostic 3D variables: PM2.5, PM10, 3 variables for interaction with photolysis and atmospheric radiation

Chemistry Package – V2.1

- 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
  - BEISv3.11 (offline reference fields, online modified)

Implementation of BEIS3 in WRFV2-Chem (Greg Frost)

Based on EPA BEIS3 for SMOKE processor



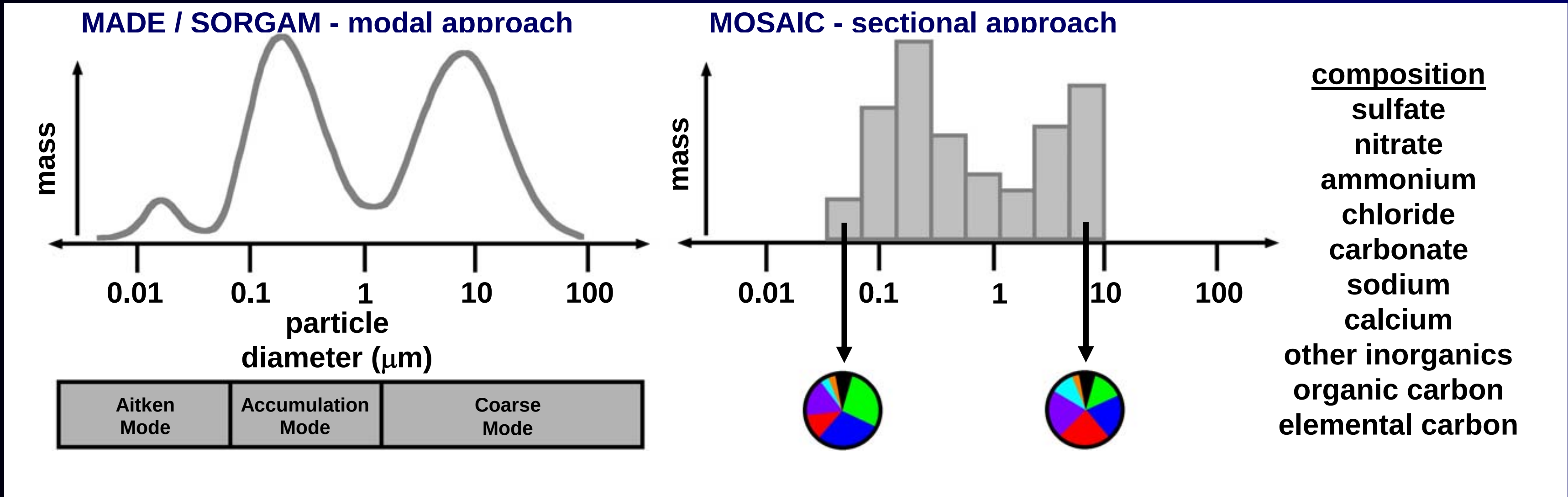
Recent Additions for WRFV2.1/Chem

- Model for Simulating Aerosol Interactions and Chemistry (MOSAIC) sectional aerosols (with 4 or 8 bins)
- Goddard radiation scheme coupled to MOSAIC aerosols

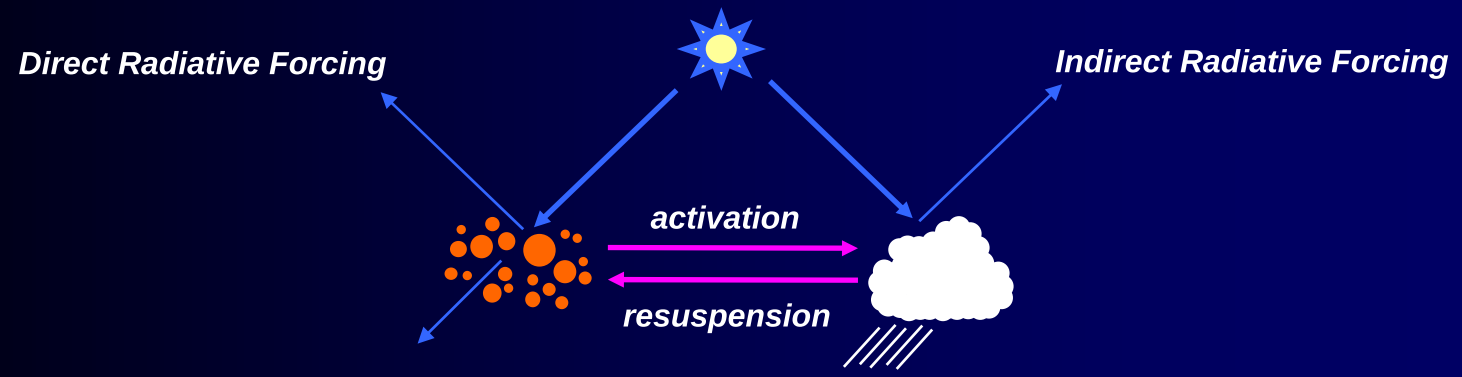
These contributions in addition to CBM-Z are from PNNL (Jerome Fast, Bill Gustafson,…)

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 interactions with meteorology



- Direct Effect *(contributions from James Barnard and Rahul Zaveri)*

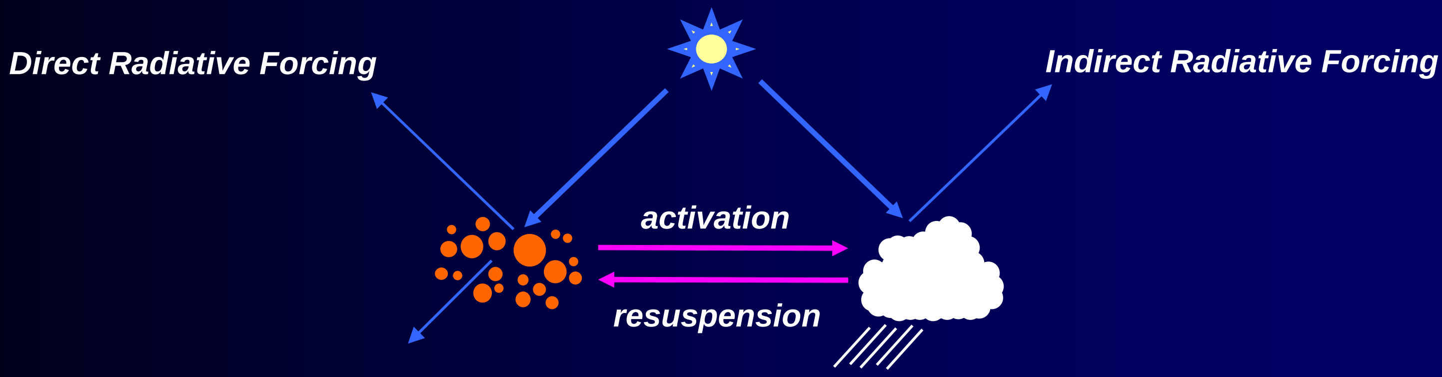
size and number distribution, composition, aerosol water → *refractive indices* → *Mie theory* → *3-D* τ_λ, ω_o, and *g* → *scattering and absorption of shortwave radiation*

<u>Currently only available for Goddard radiation scheme!</u>

Additions for WRFV2.2/Chem

- **Kinetic PreProcessor (KPP), collaboration with MPI Mainz**
- **Improved convective (non-resolved) transport**
- **Non-resolved aqueous phase chemistry, wet deposition, collaboration with NOAA/ARL/EPA in RTP**
- **2-way and 1-way nesting**
- **Cloud-aerosol interaction (indirect effect) with Lin et al. 6-class microphysics scheme (work with Greg Thompsons 6-class scheme in progress) (PNNL's doing, Steve Ghan, Jerome Fast,….)**
- **Possibility to use global boundary conditions (collaboration with Rainer Schmitz, U of Chile)**
- **Urban parameterizations (one was included in met-WRF bei Fei Chen from NCAR, but also one in the makes from Rainer Schmitz and Alberto Martilli (Madrid Spain)**
- **NMM Core**

Aerosol interactions with meteorology



Currently only for 2nd moment version of Lin et al. Microphysics

- In-Direct Effect *(contributions from Steven Ghan and Richard Easter)*

aerosol number → *aerosol activation* → *prognostic cloud droplet number, aqueous chemistry* → *cloud albedo, precipitation, cloud lifetime* → *wet removal*

$$\frac{\partial N_k}{\partial t} = -(V \bullet \nabla N)_k + D_k - C_k - E_k + S_k$$

N_k - grid cell mean droplet number mixing ratio in layer k
D_k - vertical diffusion
C_k - droplet loss due to collision/coalescence & collection.
E_k - droplet loss due to evaporation
S_k - droplet source due to nucleation

Urban parameterization from Alberto Martilli et al., as implemented by Rainer Schmitz (University of Chile) and Alberto Martilli (Madrid, Spain)

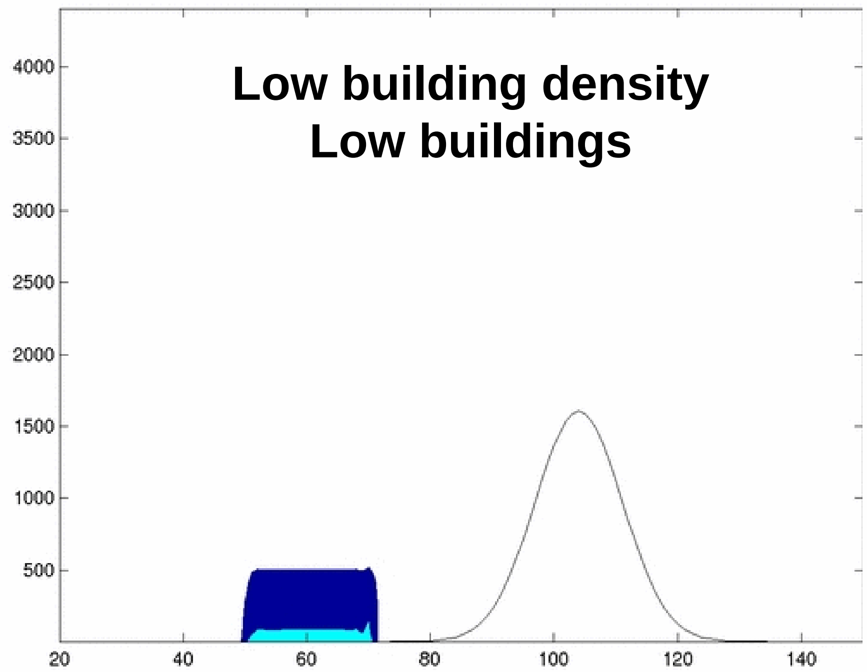
- Representation of a city by different urban classes
  - average building width
  - average street (canyon) width
  - probability of building heights

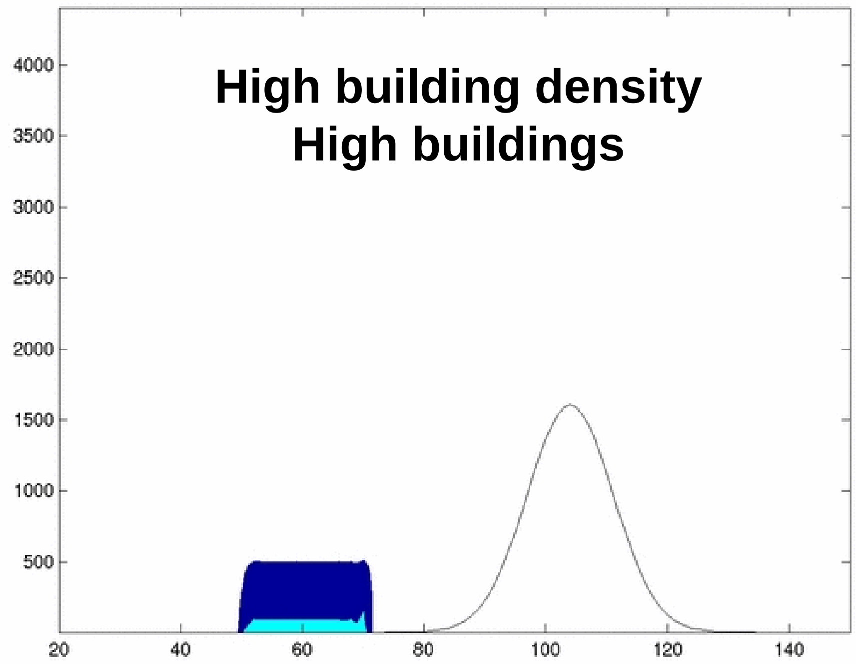
Most important effects of urban surfaces on air flow are:

– drag induced by buildings with consequent loss of momentum
– transformation of mean kinetic energy into TKE
– modifications of heat fluxes due to shadowing and radiation trapping effects

Urban parameterization – dispersion

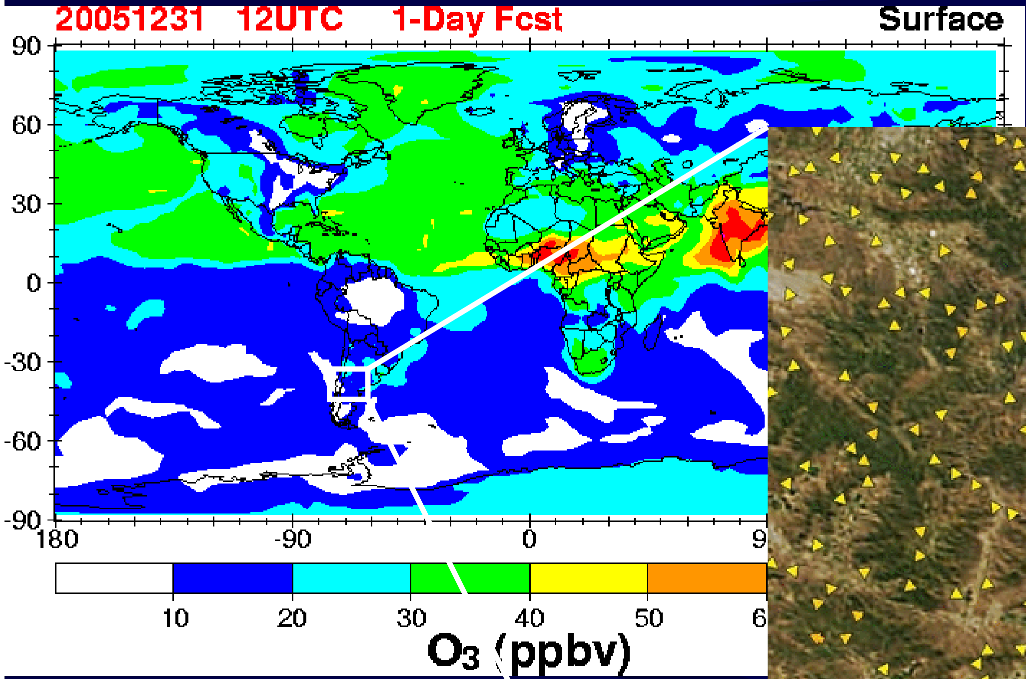
(Martilli *et al.*, 2002)





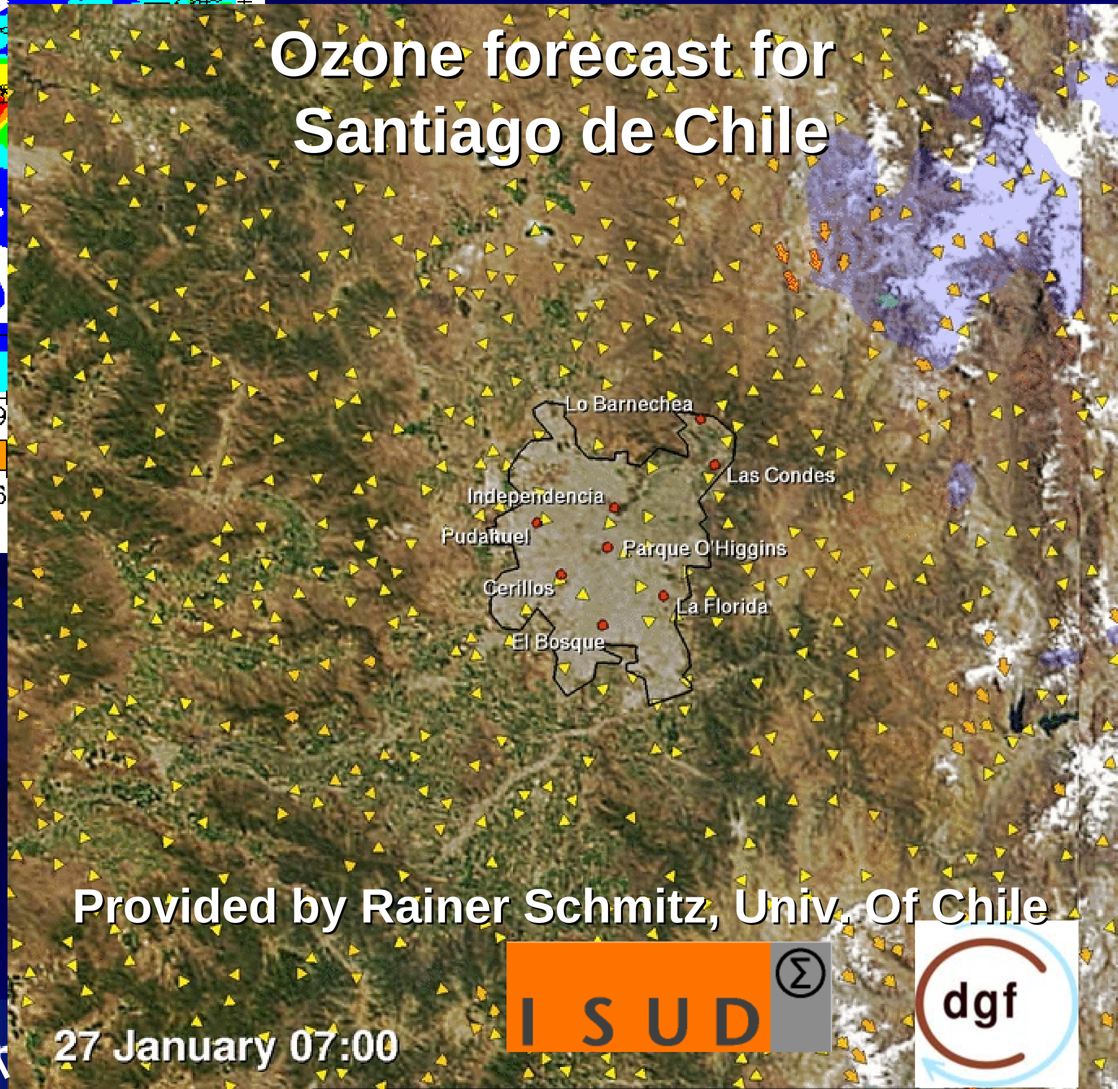
WRF idealized 2D simulation, MYJ scheme

Use of chemical data from Global Chemistry Model (GCM) for boundary conditions



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

<u>Now also available for MOZART and RAQMS</u>



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

Advantages of KPP tool

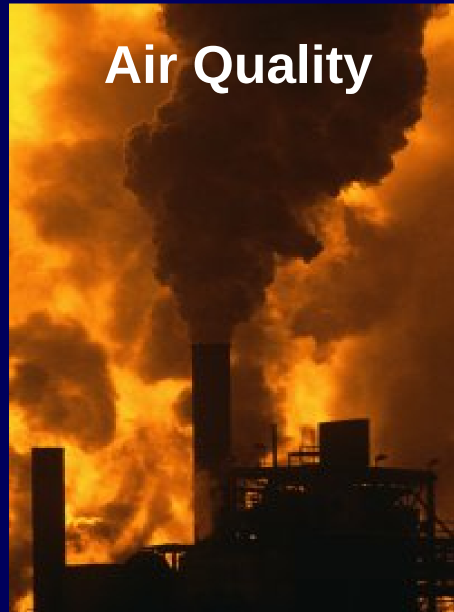
- Much less time-consuming than manual coding
- Less error prone
- Numerically reasonably efficient
- Great flexibility to
    - Update mechanisms by additional equations
    - Adjust mechanism to local conditions
    - Sensitivity studies

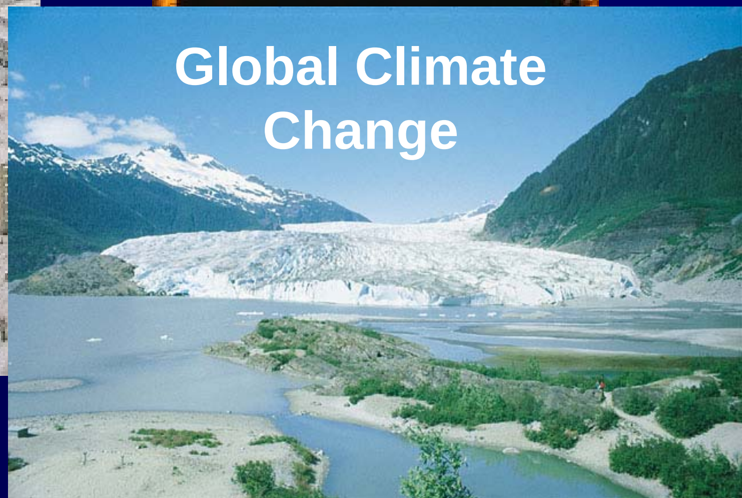
•Easy adjoint generation

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
- Aqueous phase chemistry module called from within convective routine, CMAQ module (not tested yet)
- Connected to photolysis and atmospheric radiation schemes

Current possible applications





Applications of the WRF/Chem model within ESRL/CSD

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

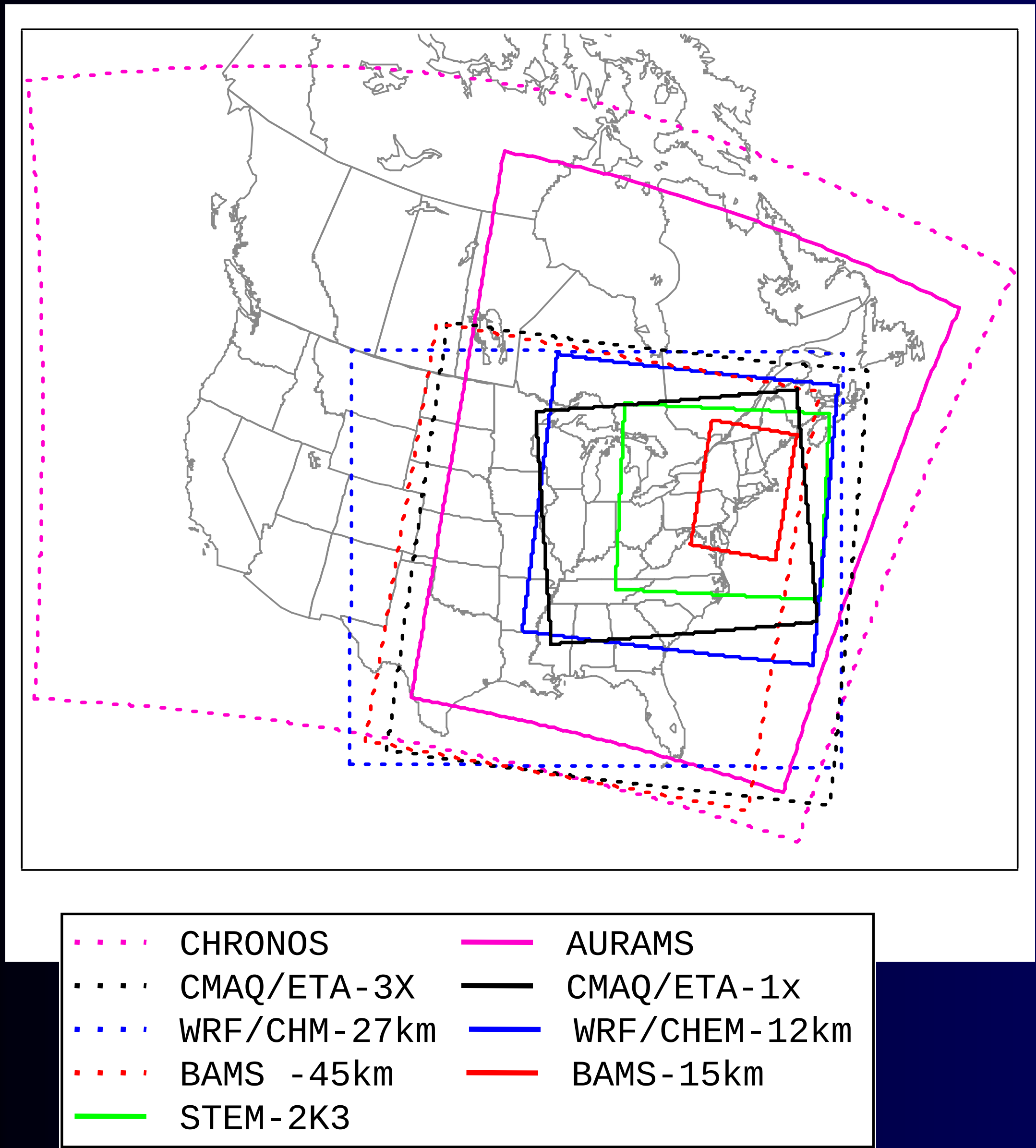
Evaluation: WRF/Chem in weather/air-quality forecast mode

- 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

Models Used in the ICARTT/NEAQS Evaluations



Model:	Anthropogenic Emission Inventory:
AURAMS - 42km CHRONOS - 21km	Canadian National Inv. (1990, 1995)
CMAQ/ETA(1x) - 12km CMAQ/ETA(3x) - 12km(*) BAMS - 45km BAMS - 15km	NEI-99, 2001, grown to 2004
WRF/CHEM-1 - 27km	NET-96
WRF/CHEM-2 - 27km WRF/CHEM - 12km(*) STEM(2K3) - 12 km	NEI-99

Red indicates PM2.5 forecasts available
(*) Indicates a retrospective run

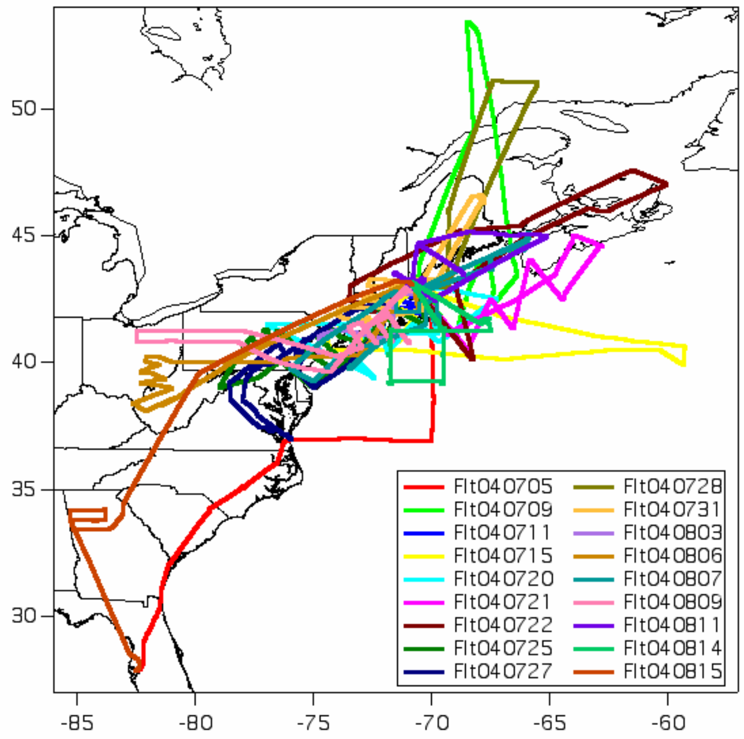
Web-page for NOAA P3 and Ron Brown model comparisons: http://www.al.noaa.gov/ICARTT/modeleval/

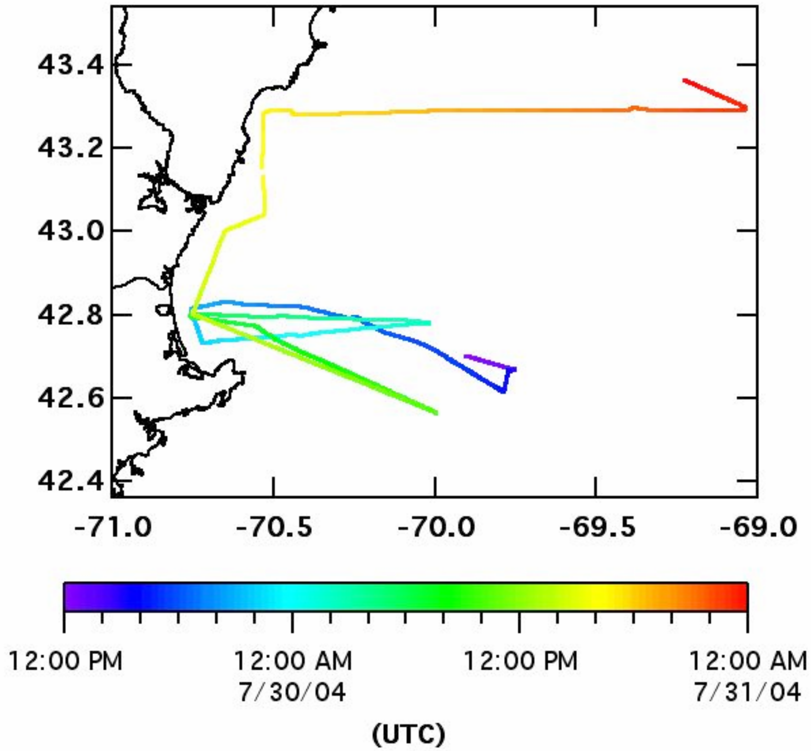
NOAA Aeronomy Lab, Theoretical Aeronomy Division

ICARTT/NEAQS 2004 - Air Quality Forecast Model Verification Project (Stu McKeen)

NOAA P3 Summary Statistics

Ron Brown, 7/07/04 - 7/23/04
Ron Brown, 7/27/04 - 8/12/04





Flight by flight vertical profiles and horizontal transect

This page maintained by: Stu McKeen
NOAA AERONOMY LABORATORY

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/

Statistics for 8 Air Quality Forecast Models with 342 AIRNOW O_3 monitors

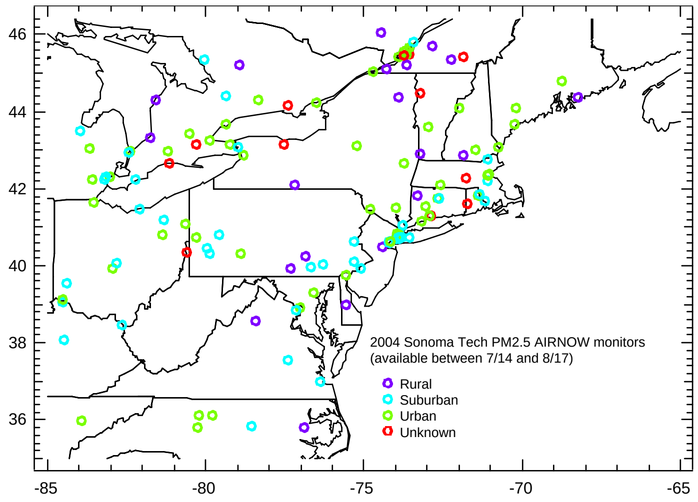
(7/14/04 through 8/17/04 - 34 days)

(7/14/04 through 7/29/04 - 16 days)

Statistics for maximum 8-hr averages, (00Z forecasts).
Medians of 342 monitor co mparisons

Date of WRF/Chem Run	Institute, model, horiz. resolution	r coefficent	Mean bias ppbv	RMSE (ppbv)	Skill (%)
	MSC Canada, CHRONOS, 21km (2004 real-time)	0.68	17.0	23.2	16%
	MSC Canada, AURAMS, 42km (2004 real-time)	0.54	5.9	16.2	27%
	U of Iowa, STEM, 12km (2004 real-time)	0.60	26.4	31.	2%
	CMAQ/ETA, 12 km (2004 real-time)	0.63	13.4	17.9	24%
8/04	WRF/Chem – V1.3 – 27km	0.67	14.3	20.9	24%
11/04	WRF/Chem – V2.0 – 27km	0.73	3.4	11.6	61%
3/05	WRF/Chem – V2.0 – 12km	0.67	11.9	16.6	31%
5/05	WRF/Chem – V2.0.3	0.72	12.8	17.0	30%
5/05	WRF/Chem – V2.1.2	0.72	11.5	16.3	30%
10/06	WRF/Chem – V2.1.2x	0.82	6.4	11.2	73%
1/07	WRF/Chem – V2.2	0.83	3.3	9.8	81%

PM2.5 Monitors within the AIRNow network



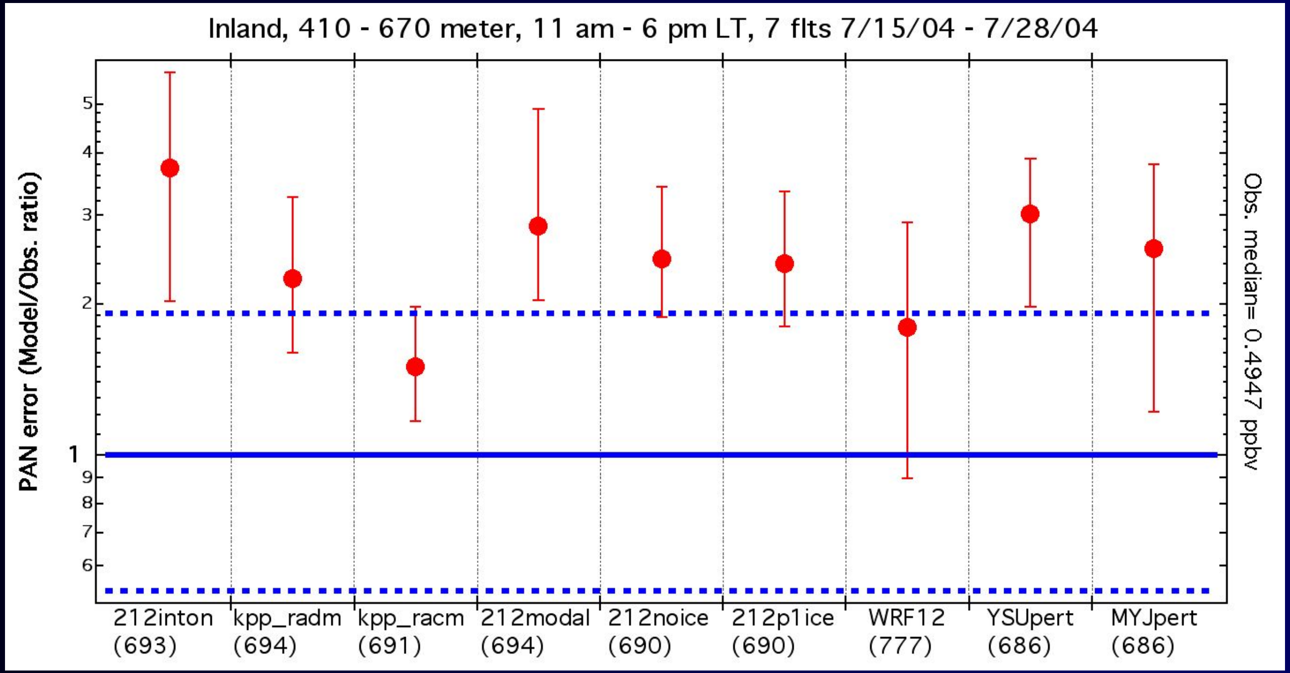
- ~120 TEOM monitors
- 10 am to 6 pm LDT averages
- No spatial interpolation
- Statistics done for log-transformed PM2.5
- Only days with complete model overlap

Statistics for 6 Air Quality Forecast Models with 118 AIRNOW PM2.5 monitors (7/14/04 through 8/17/04 - 34 days)

Statistics for 14Z to 22Z 8-hr av erages, based on 00Z forecasts only.
Medians of 118 monitor co mparisons

Institute, model, horiz. resolution	r coefficent	Modl/Obs ratio	RMSE (factor)	Skill (%)
NOAA FSL, WRF/Chem-1, 27km	0.42	1.17	2.19	33%
NOAA FSL, WRF/Chem-2, 27km	0.65	0.79	1.79	64%
MSC Canada, CHRONOS, 21km	0.67	0.77	2.14	53%
MSC Canada, AURAMS, 42km	0.49	0.85	2.16	58%
U of Iowa, STEM, 12km	0.65	1.12	1.95	70%
CMAQ/ETA, 12 km	0.65	0.75	2.01	61%
6-model Ensemble	**0.75**	**0.86**	**1.76**	**75%**

Comparison of PAN Forecast with NOAA -P3 aircraft data



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WRFV2.2

Key:

212inton - V2.1.2, Pegasus - CBMZ, no convective subgrid transport

Kpp_radm - V2.1.2, RADM2, subgrid convection on, subgrid photol. reduc. On
ice contribution to photolysis reduction in resolved clouds (1. cloud equiv)

Kpp_racm - V2.1.2, RACM, subgrid convection on, subgrid photol. reduc. On
ice contribution to photolysis reduction in resolved clouds (1. cloud equiv)

212modal - V2.1.2, RADM2, subgrid convection off, subgrid photol. reduc. off

212noice - V2.1.2, RADM2, subgrid convection on, subgrid photol. reduc. off
no ice contribution to photolysis reduction in resolved clouds

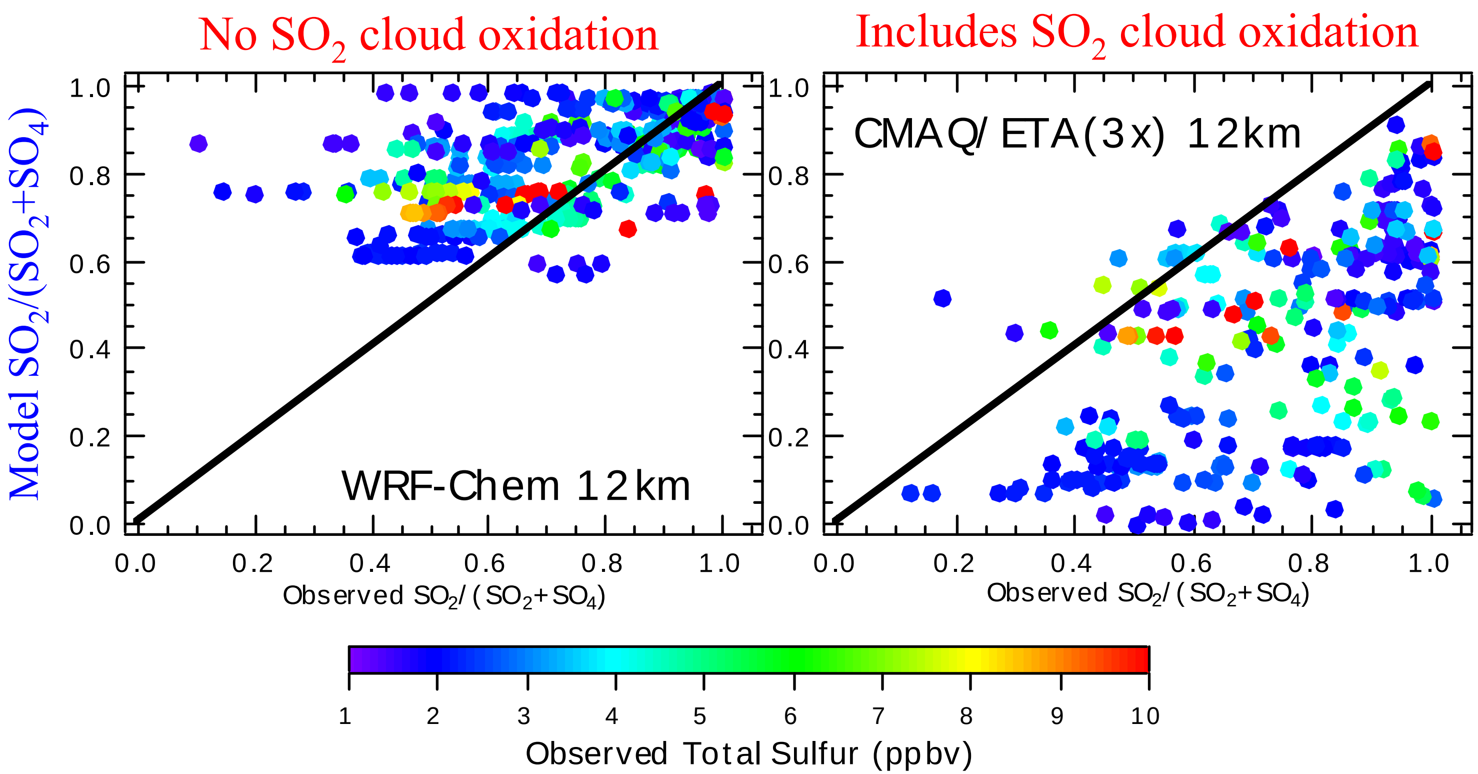
212p1ice - V2.1.2, RADM2, subgrid convection on, subgrid photol. reduc. off
ice contribution to photolysis reduction in resolved clouds (.1 cloud equiv)

WRF12 - V2.0.3, RADM2, 12 km res. YSU PBL (convection on, no subgrid photol reduc.)

YSUpert - V2.0.3, RADM2, 27km res., YSU PBL scheme (“ “ “)

MYJpert - V2.0.3, RADM2, 27km resolution, MYJ PBL scheme (“ “ “)

Comparing SO_2 oxidation rates, Models versus Obs.

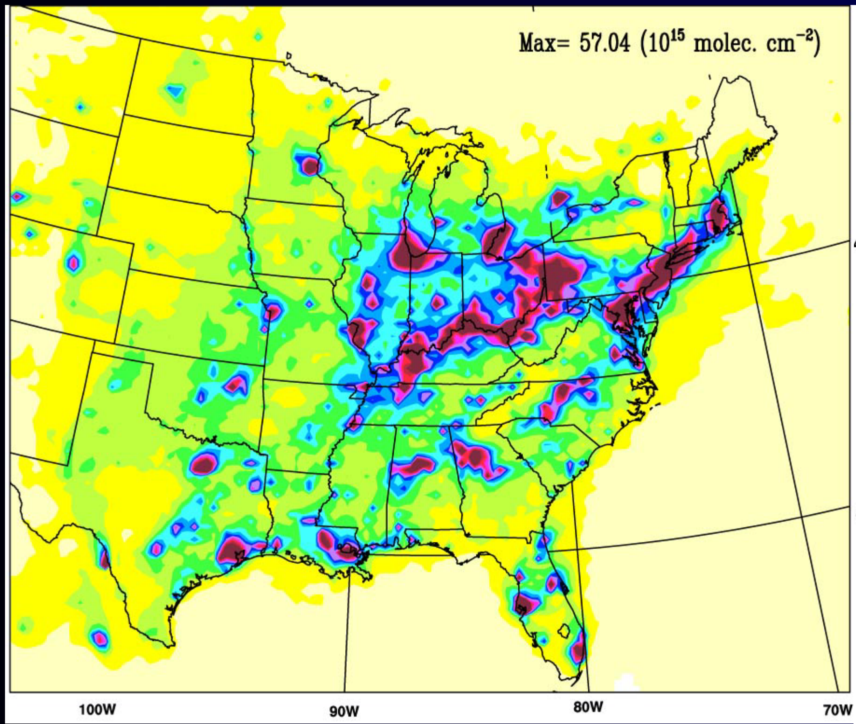


Models without cloud oxidation under-predict SO_4 and SO_2 oxidation
Models with cloud oxidation over-predict SO_4 and SO_2 oxidation

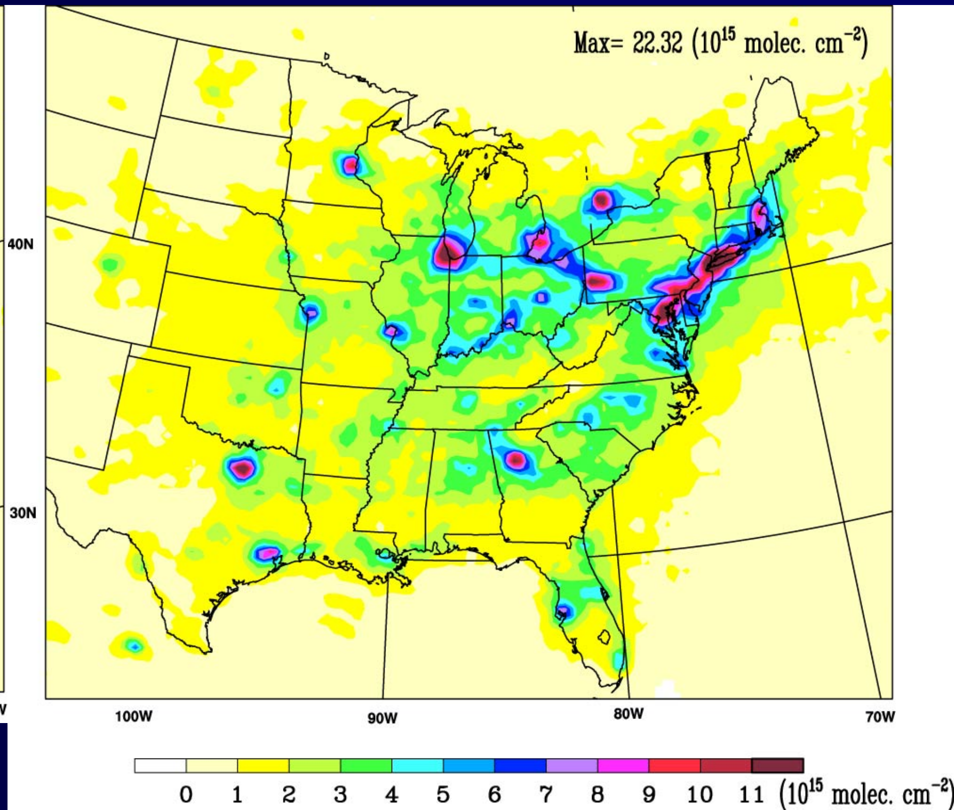
Spatial Distribution of NO_2 Columns
(Si-Wan Kim et al., GRL, 2006)

Summer 2004 (June-August) Averages

WRF/Chem - NEI 99 v3 emissions



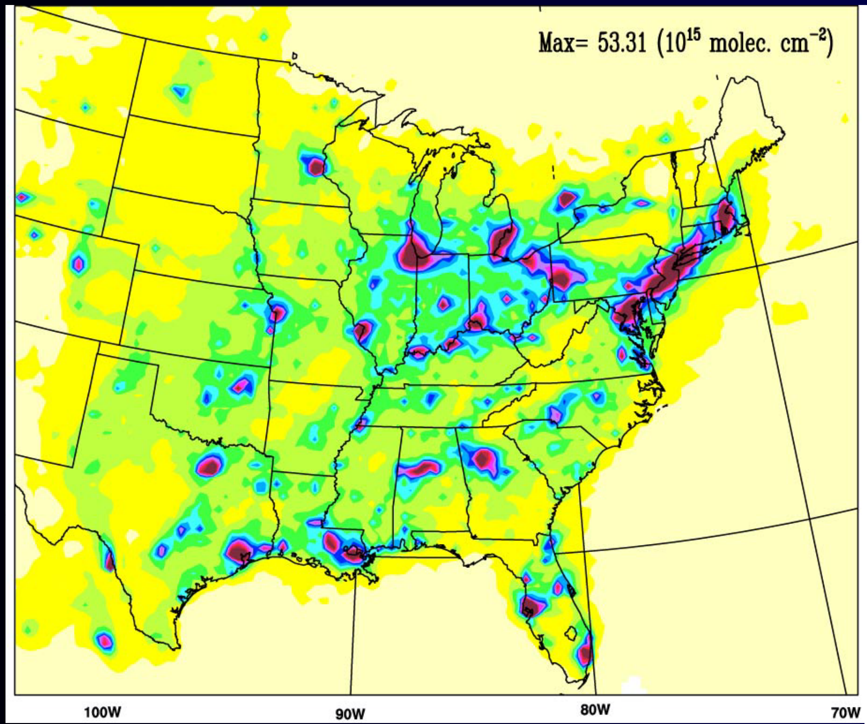
SCIAMACHY satellite observations



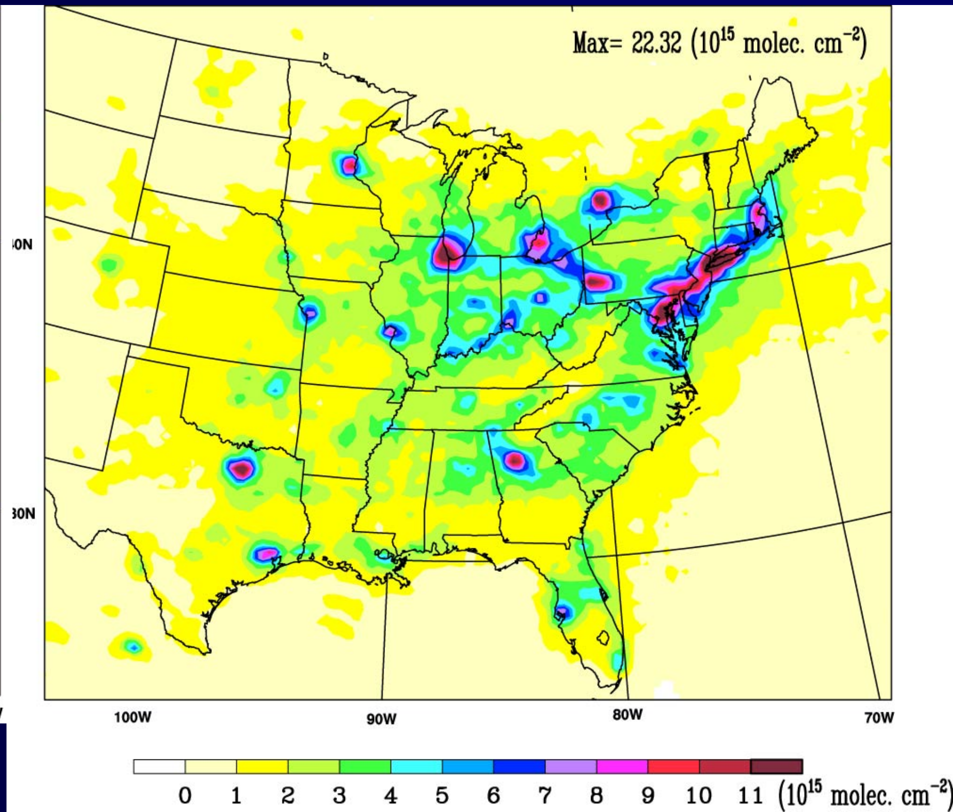
Spatial Distribution of NO_2 Columns
(Si-Wan Kim et al., GRL, 2006)

Summer 2004 (June-August) Averages

WRF/Chem - Updated emissions - CEMS monitors at ~ 1000 stacks



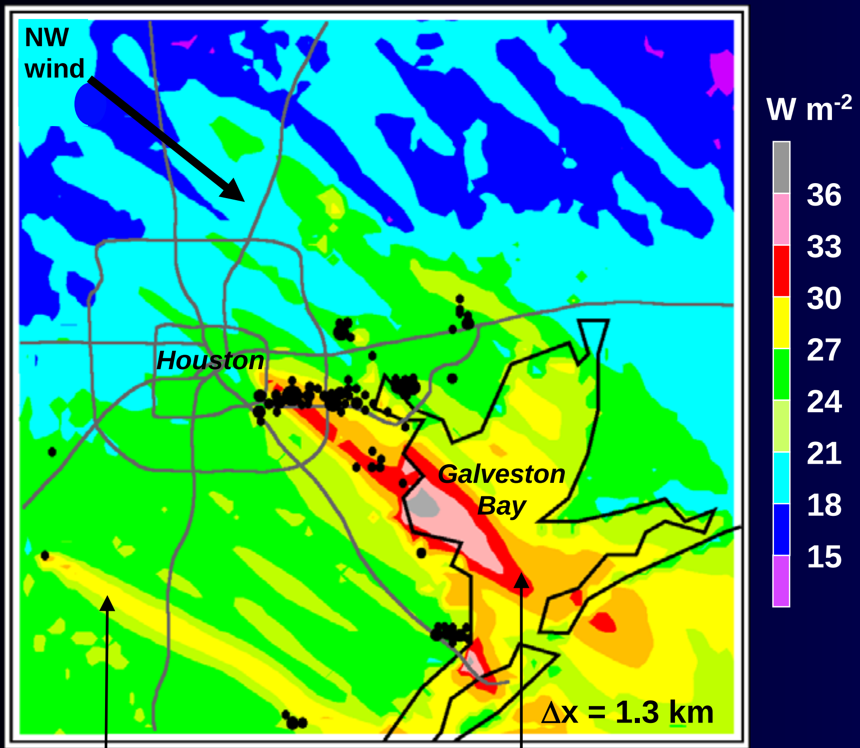
SCIAMACHY satellite observations



TexAQS 2000 – DRY RUN

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

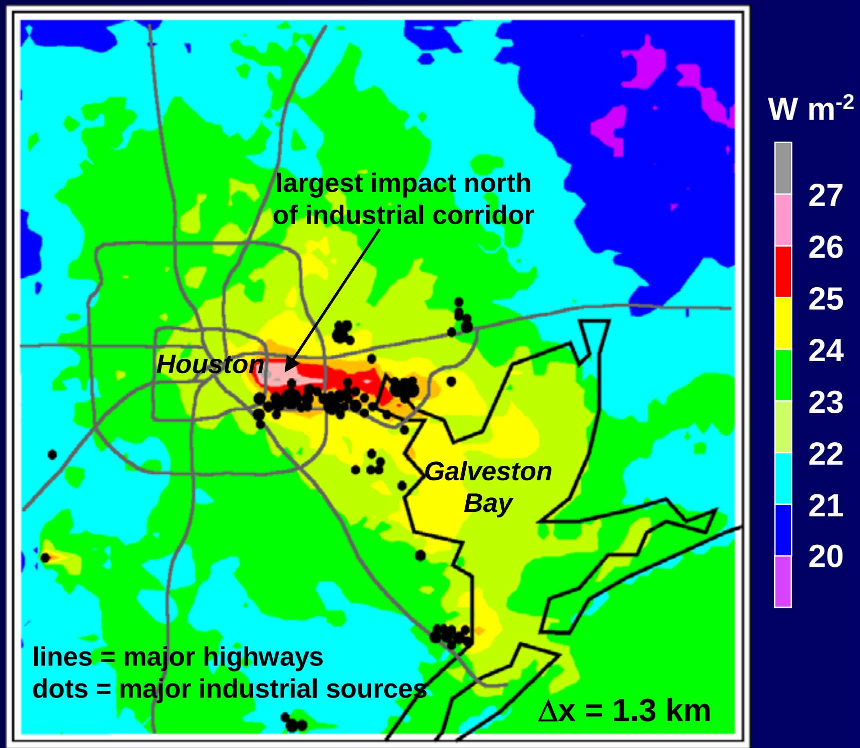
Instantaneous Aerosol Radiative Forcing
Noon, August 31, 2000



impact of sulfate from power plant

impact of organic and elemental carbon from urban and industrial sources

Average Aerosol Radiative Forcing
August 28 - 1 September, 2000

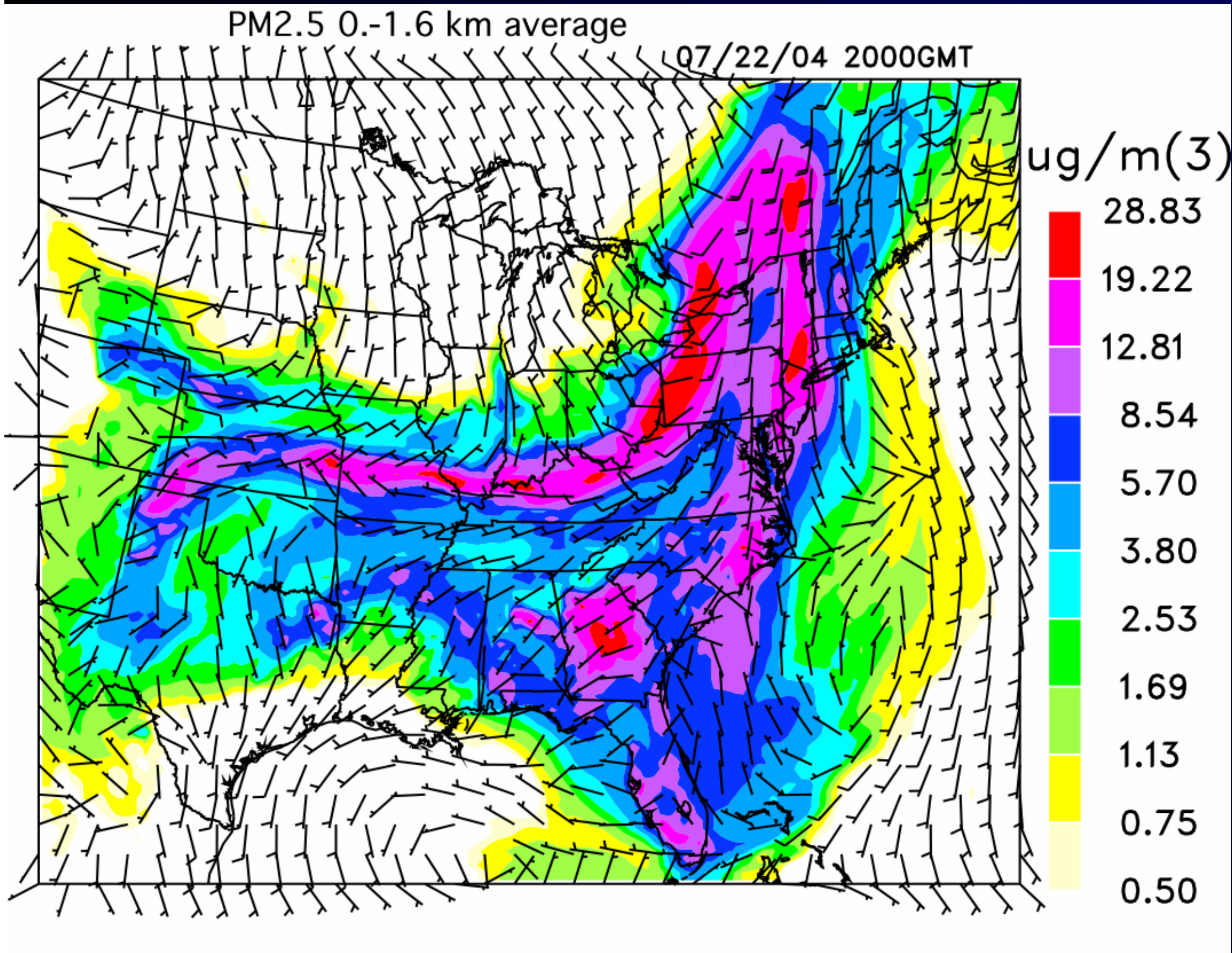


120 km
(typical GCM Δx = 100 km)

- ➔ Impact of anthropogenic particulates are a major uncertainty in GCMs
- ➔ Large spatial variations in particulates and the resulting radiative forcing over urban areas are not resolved by Global Climate Models (GCMs)

PM2.5 predictions – One case only

Average over lowest 1.6km

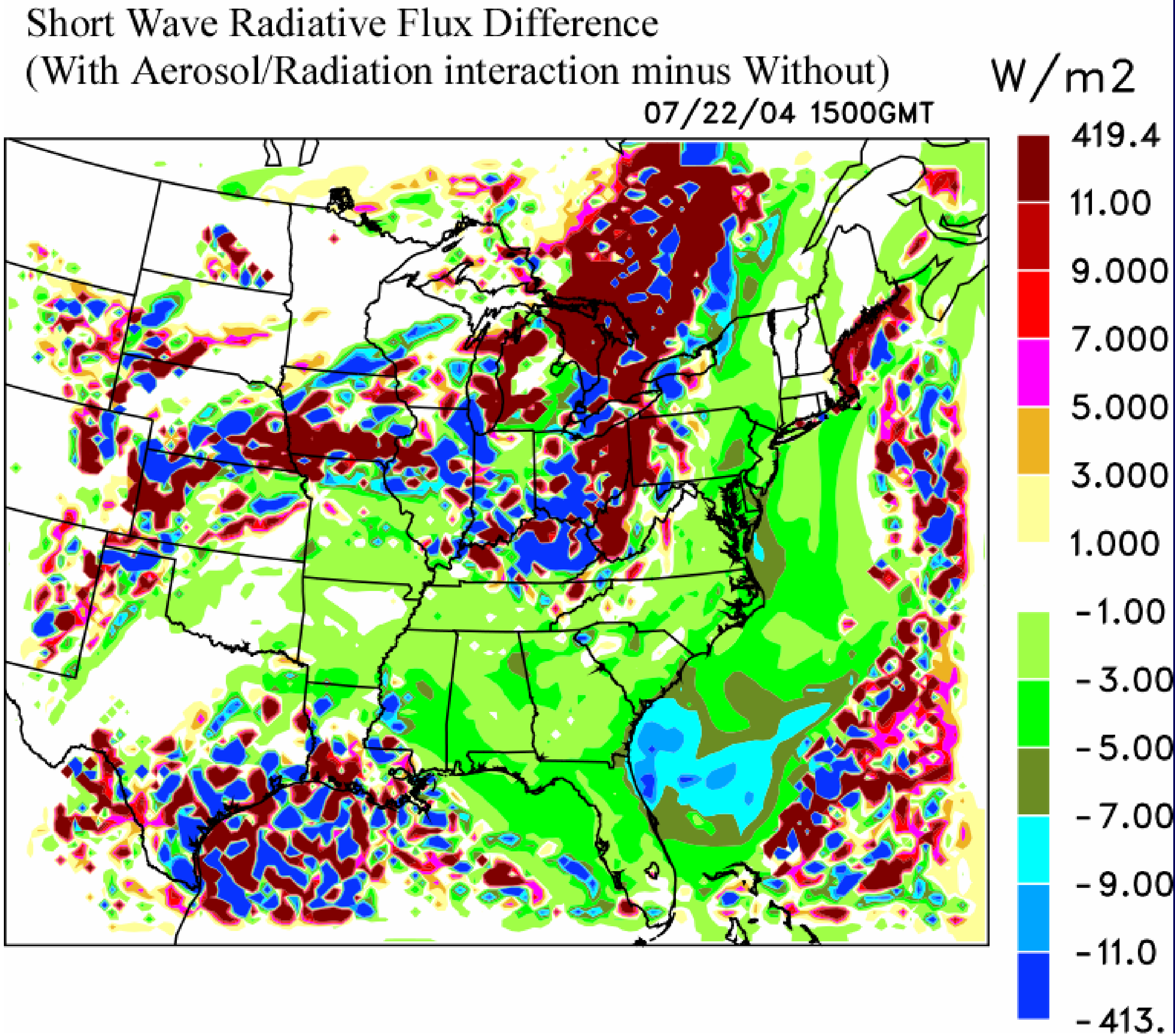


32 hr forecast

Full physics,

Lin et al. Microphysics,
Grell/Devenyi convection

Aerosol/Radiation feedback: Short Wave radiative Flux Difference using different microphysics scheme



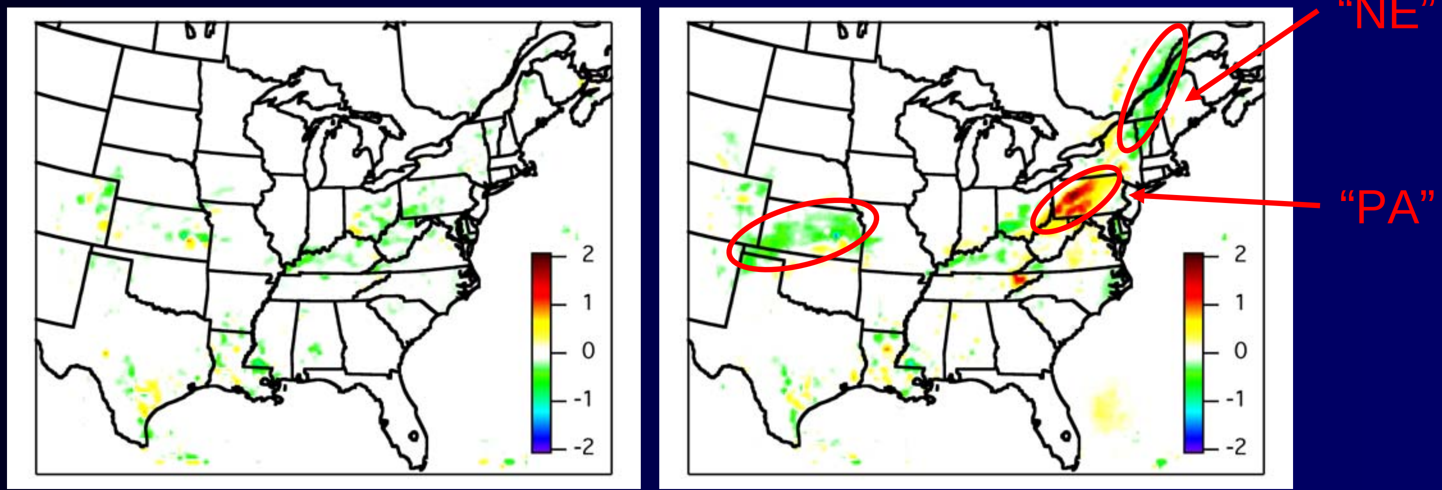
15 hr forecast

Aerosol-Radiation Effects on 2m-Temperature

Contribution from Serena Chung

$\Delta T_{@2m}$ (^{o}C)

Scattering Only | With Absorption



07/23/2004 18:00:00 UTC

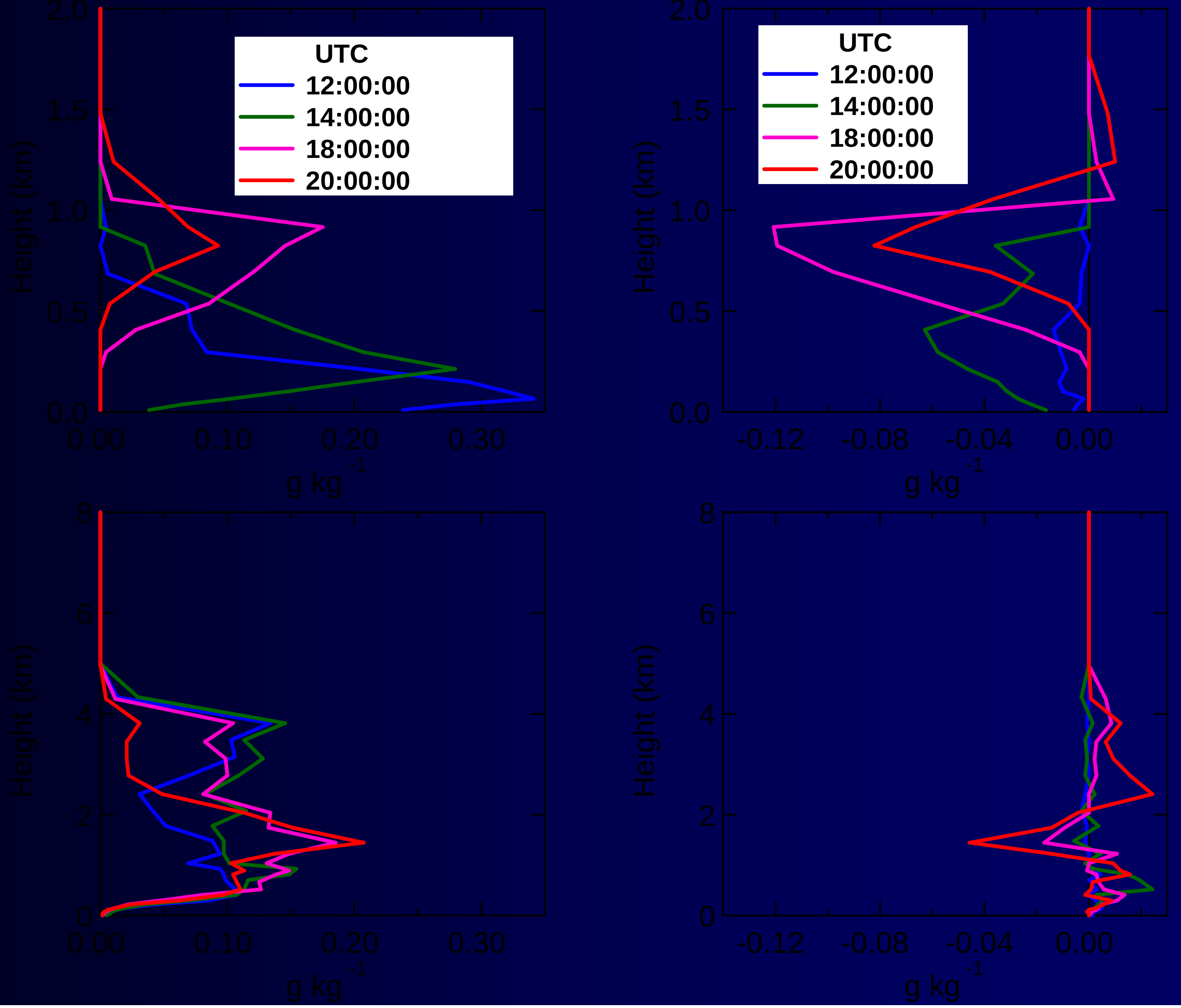
Vertical Distribution of Liquid Water

Liquid Water Content
(no feedback)

Δ Liquid Water Content
(with absorption)

at "PA"

at "NE"



07/23/2004

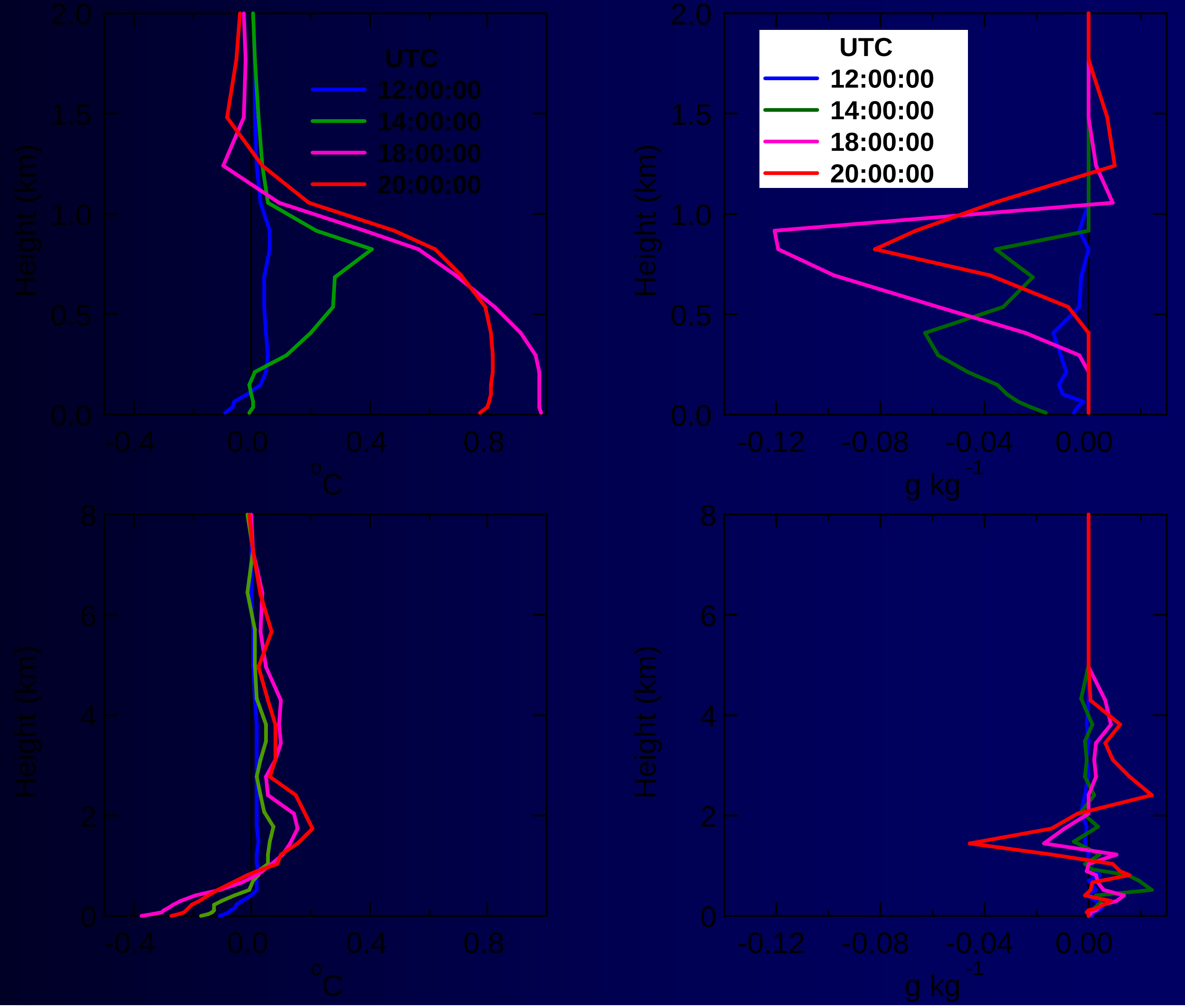
Vertical Distribution of ΔT

ΔT
(with absorption)

Δ Liquid Water Content
(with absorption)

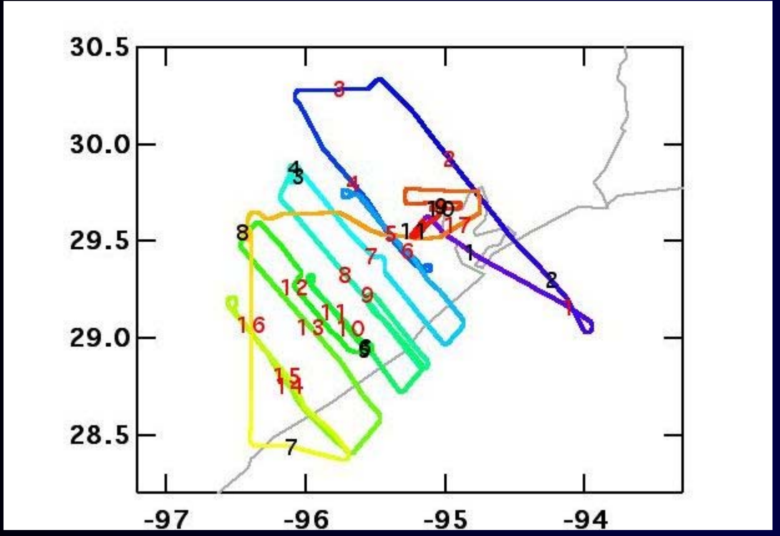
at “PA”

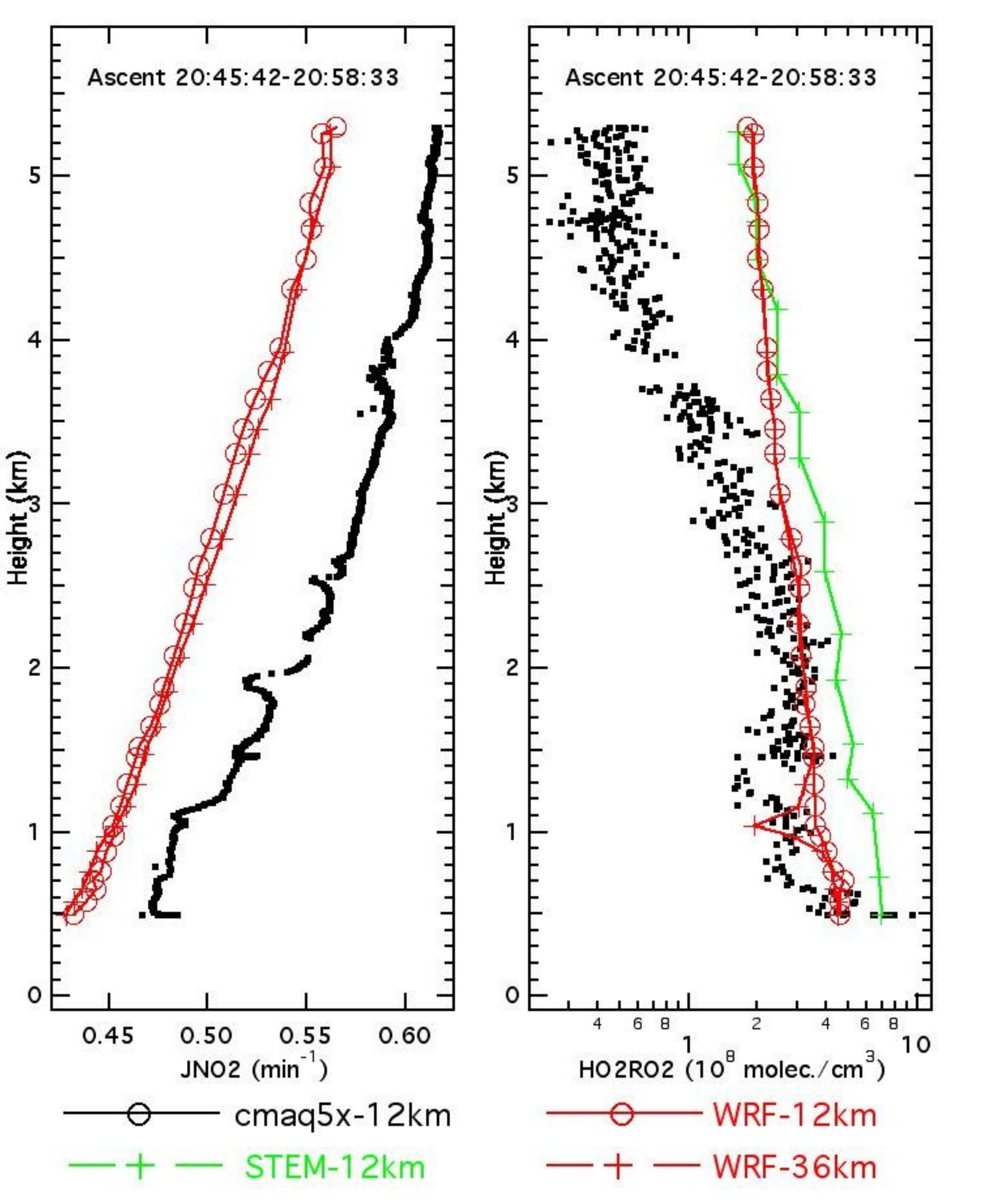
at “NE”



07/23/2004

Texas 2006 – aircraft comparisons





Some conclusions from research applications for WRF/Chem:

AQ Forecasting:

Steady improvements in forecasting O_3 and $PM_{2.5}$ aerosol

WRF/Chem is highly competitive compared to other AQ models

Research within CSD:

Used in Satellite studies of Anthropogenic Emission Changes

Aerosol-Radiation-Meteorology Interactions

Additional Process Studies related to PBL parameterizations, Chemistry, and Aerosols

Next in line-up for inclusion into WRF/Chem (ARW and NMM)

- CMAQ modules: for compatibility with EPA's CMAQ model: Carbon Bond 5 chemical mechanism, and MADRID sctional aerosol module (collaboration with NCSU)
- Offline version (Indo-US project)
- Sasha Madronich's latest, fast photolysis scheme (NCAR)
- Global versions (ARW? NMM?)
- SMOKE emissions model
- MEGAN biogenic emissions (NCAR)
- Smoke/Fire plume model

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

- More aerosol modules
- Dust/sea-salt parameterizations
- More choices for "interactive" parameterizations (like radiation or microphysics schemes that allow for feedback from chemistry to meteorology)

Future development plans, as brought forth in WRF Research and Applications Board document:

- Computational efficiency (monotonic, conserving advection), possibly other technical changes to WRF-CI
- ***Advanced data assimilation methods***
- Expansion of KPP capabilities
- Implementation of necessary steps and research to be able to use the modeling system for design of observational networks (use of OSE's and OSSE's)
- Coupling to other modeling systems (ocean, agriculture, biology,…)