Evaluation of real-time air quality and weather predictions using WRF-Chem

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Overview

- Real-time model set-up
  - Discuss same domain for several field programs
- Model evaluation results
  - Meteorological evaluation
  - Chemistry model evaluation
- Current modeling activities at NOAA

Field Programs

ICARTT/NEAQS 2004*

- AIRNow O_3 monitors (~340)
- AIRNow PM2.5 monitors (~120)
- Speciation Trends Network (72 monitors)
- NOAA P3 Aircraft
- NOAA DC-3 Airborne Ozone Lidar
- NOAA Research Vessel Ronald H. Brown

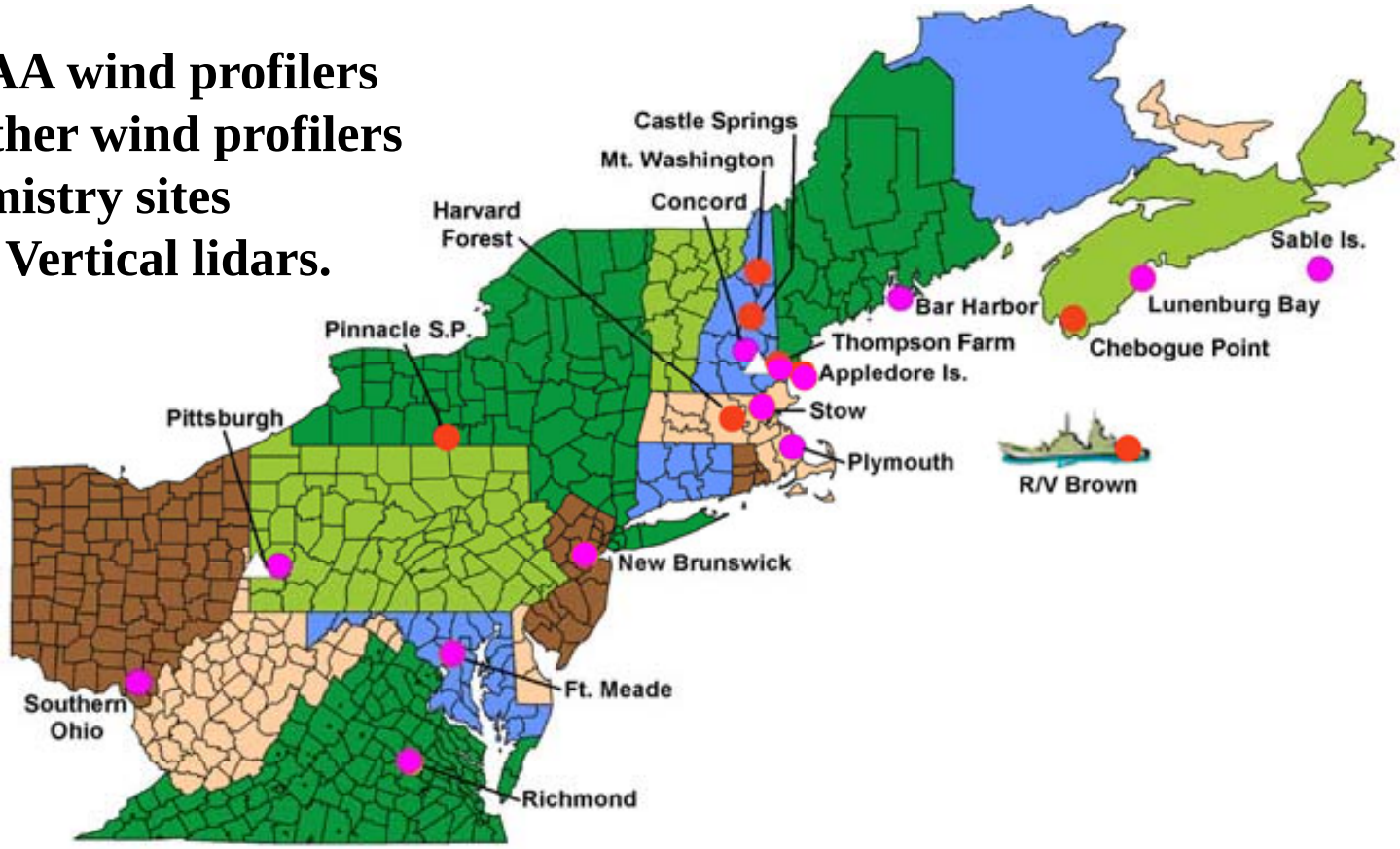
*International Consortium for Atmospheric Research on Transport and Transformation / New England Air Quality Study

RV Ronald H. Brown

ICARTT/NEAQS 2004

2004 surface network

Pink: NOAA wind profilers
Yellow: Other wind profilers
Red: Chemistry sites
Triangles: Vertical lidars.

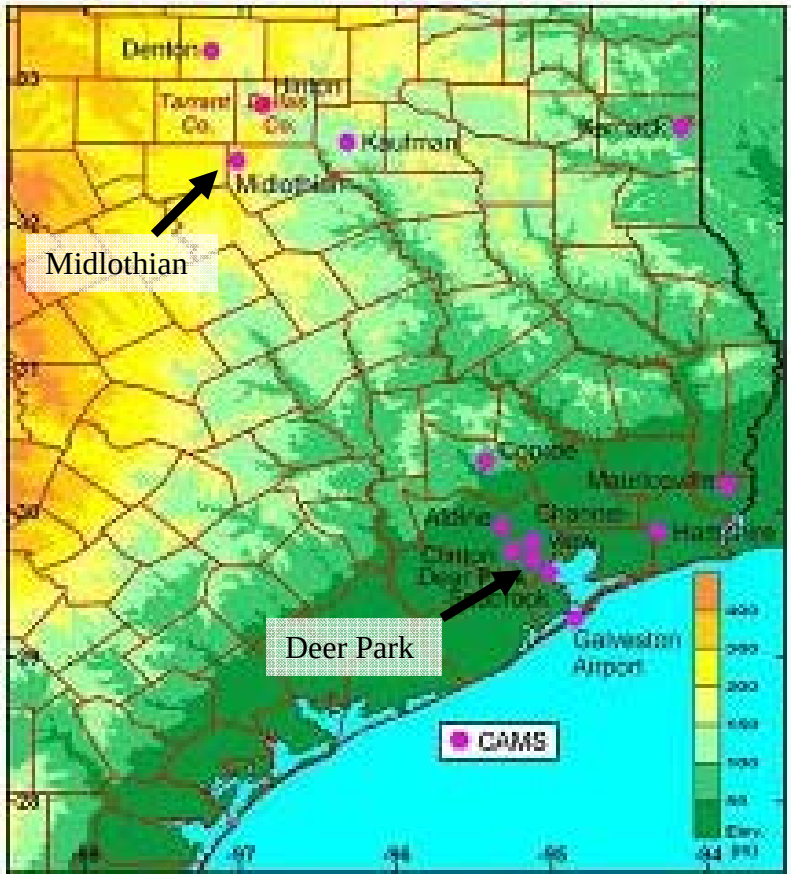


TEXAQS 2006
Surface Meteorology and Chemistry Obs.

http://www.etl.noaa.gov/programs/2006/texaqs/verification/

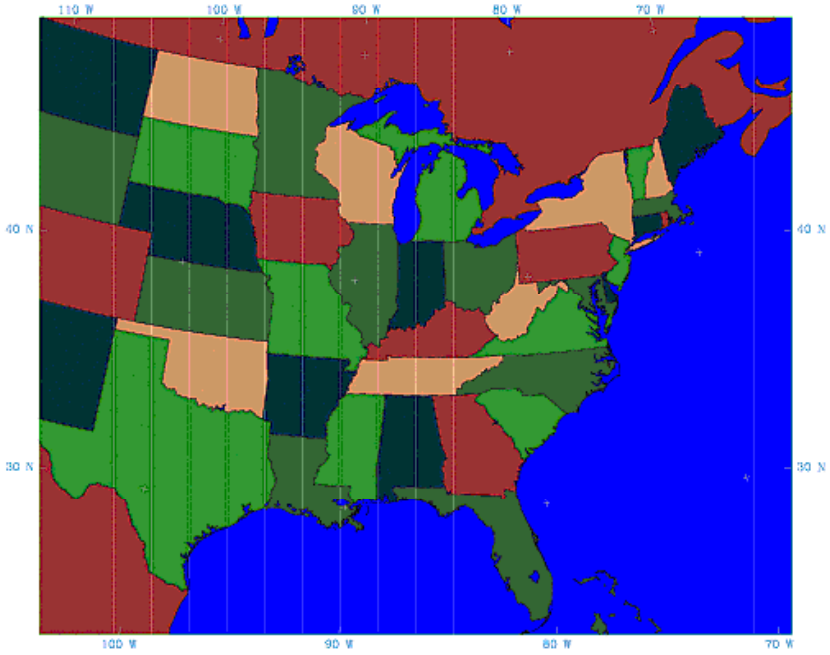
- Surface Meteorology:
  wind speed and direction,
  temperature,
  humidity,
  pressure,
  precipitation,
  solar and net radiation

- Surface Chemistry:
  Ozone: O_3,
  Fine particles: PM2.5,
  Nitrous Oxides: NO_x,
  Carbon Monoxide: CO,
  Sulfur Dioxide: SO_2



2004/2006 real time forecast domain

- 27-km horizontal grid spacing, 110 x 134 x 35 grid points, dt = 120 s
  - ~ 1.5 h on 64 intel processors for 36 h forecast
  - Made available online for immediate use
- Historical - originally used in NEAQS 2002 to compare w/ MM5-Chem)



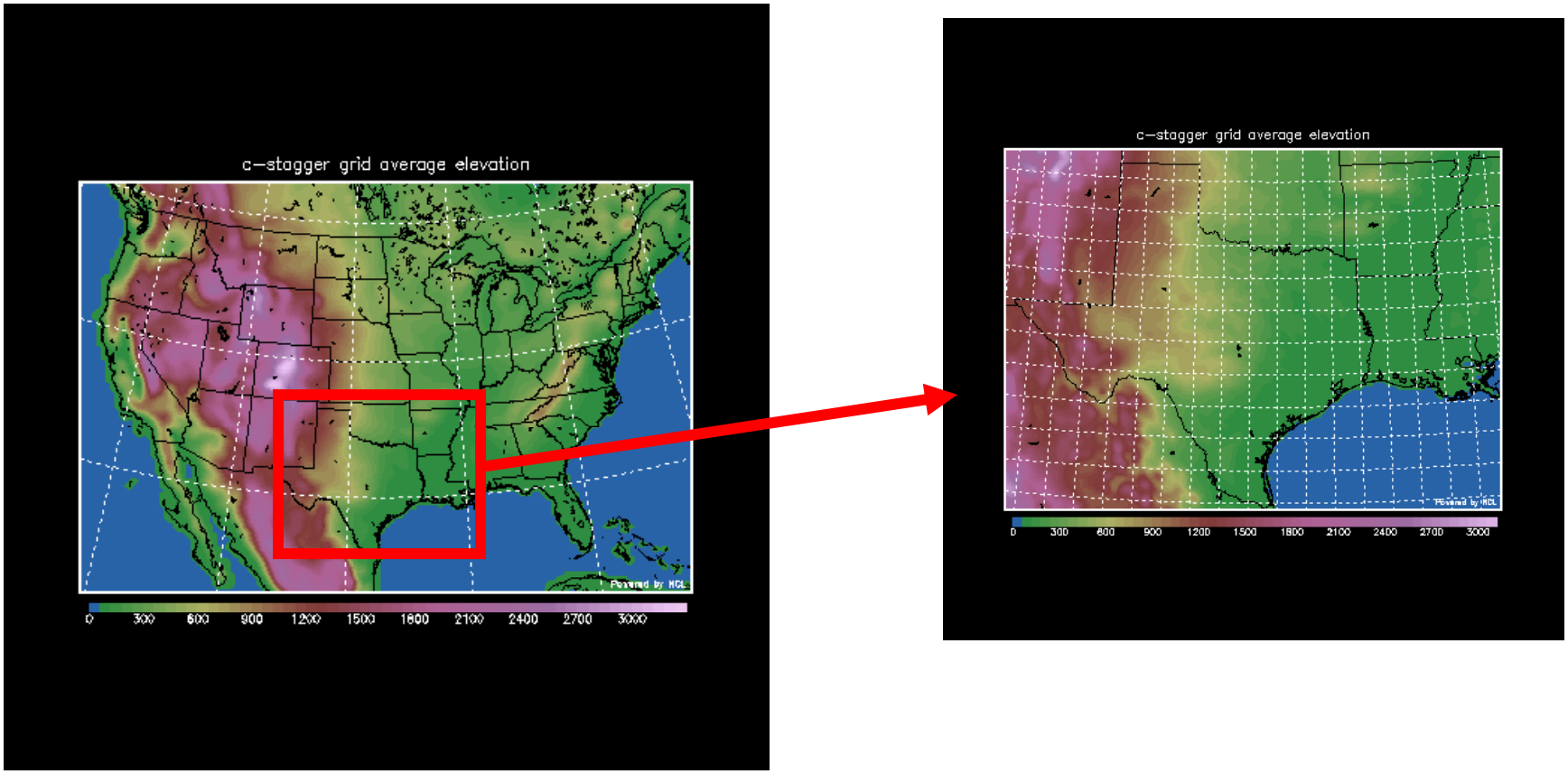
2004/2006 real time WRF-Chem settings

- Table 1. Model configuration options and parameterizations used in the WRF-Chem real-time air quality forecasts using 27-km horizontal grid spacing.

• Advection scheme	5^{th} horizontal /3^{rd} vertical
• Microphysics	NCEP 3-class simple ice
• Longwave radiation	RRTM
• Shortwave radiation	Dudhia
• Surface layer	Monin-Obukhov (Janjic Eta)
• Land-surface model	RUC_LSM (Smirnova et al. 1997)
• Boundary layer scheme	Mellor-Yamada-Janjic 2.5 TKE
• Cumulus parameterization	Grell and Devenyi, 2002
• Chemistry option	RADM2 (Stockwell et al. 1990)
• Dry deposition	Weseley, 1989
• Biogenic emissions	BEIS 3.11 (v 2.03)
• Anthropogenic Emissions	NEI 1999 v 3.0
• Photolysis option	Madronich, 1987
• Aerosol option	MADE/SORGAM

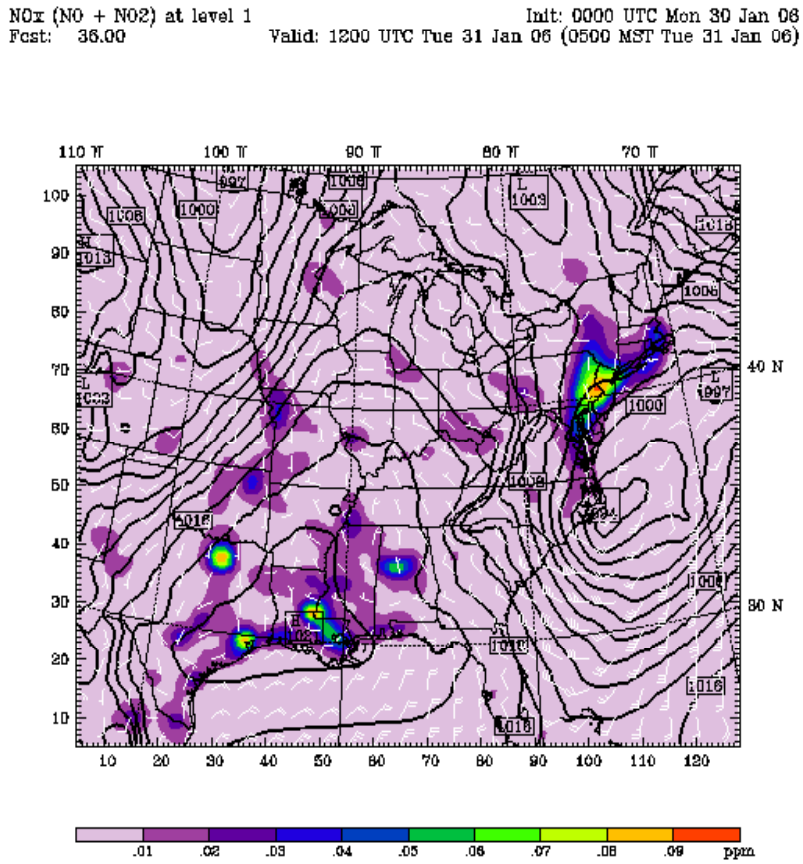
Real Time AQ Forecast Domain

- Also ran 12km domains for each field program
  - e.g., 12-km nested domain used in TEXAQS 2006



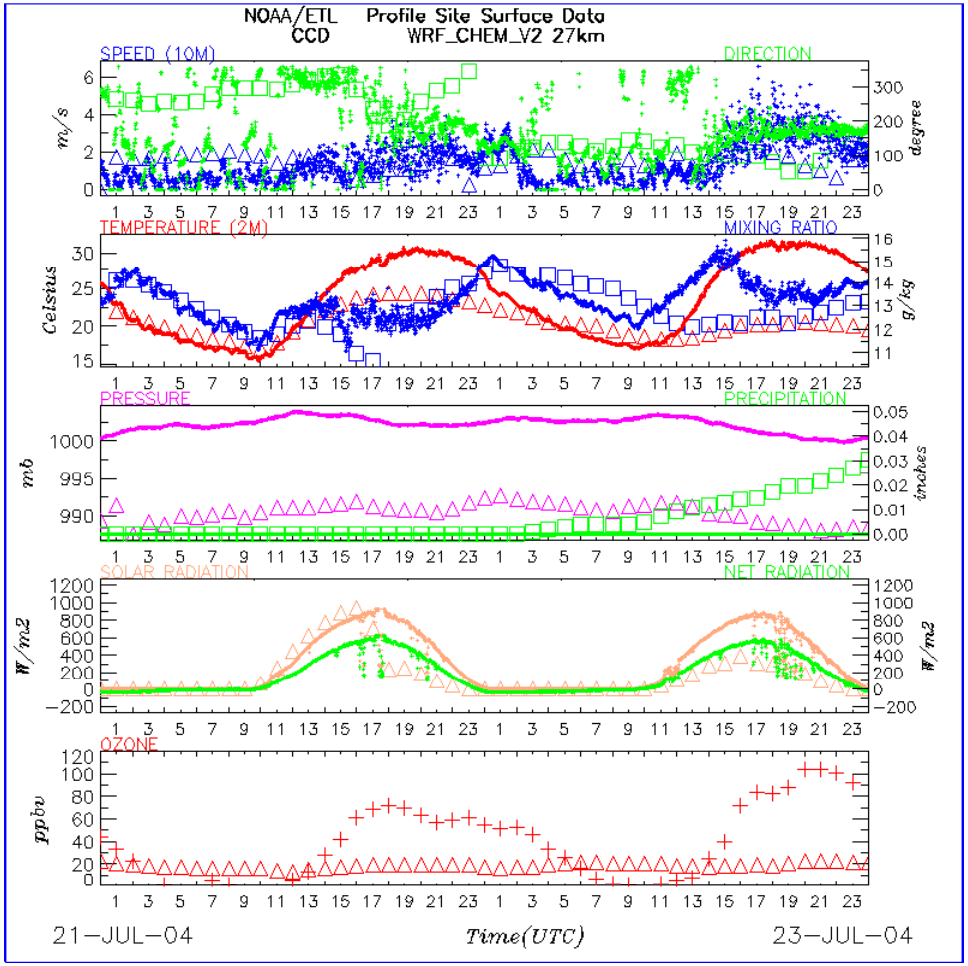
Real time WRF-Chem

- Data made available in real time via Web
  - Surface fields
    - MP2.5
    - Surface winds
  - Also plots of:
    - Ozone, CO, etc.
    - Precipitation, standard pressure levels met., clouds



Real time WRF-Chem

- Other example of data available on web pages
  - –Many standard meteorological fields
  - –Some chemical fields
  - –Useful for meteorological evaluation



Observations from at Concord, NH

Real-time WRF-Chem

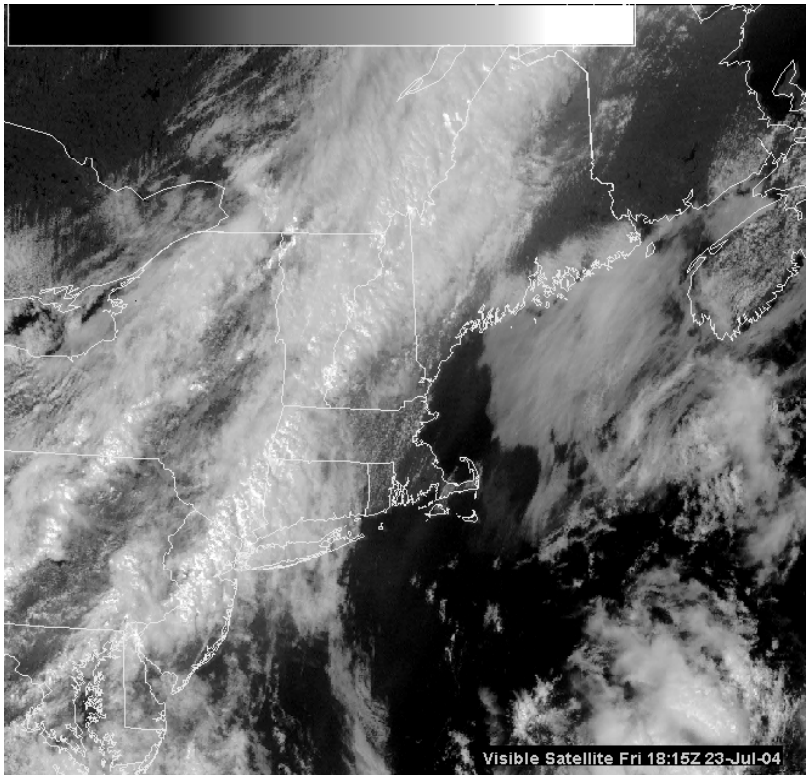
- Meteorological Evaluation (Jim Wilczak)

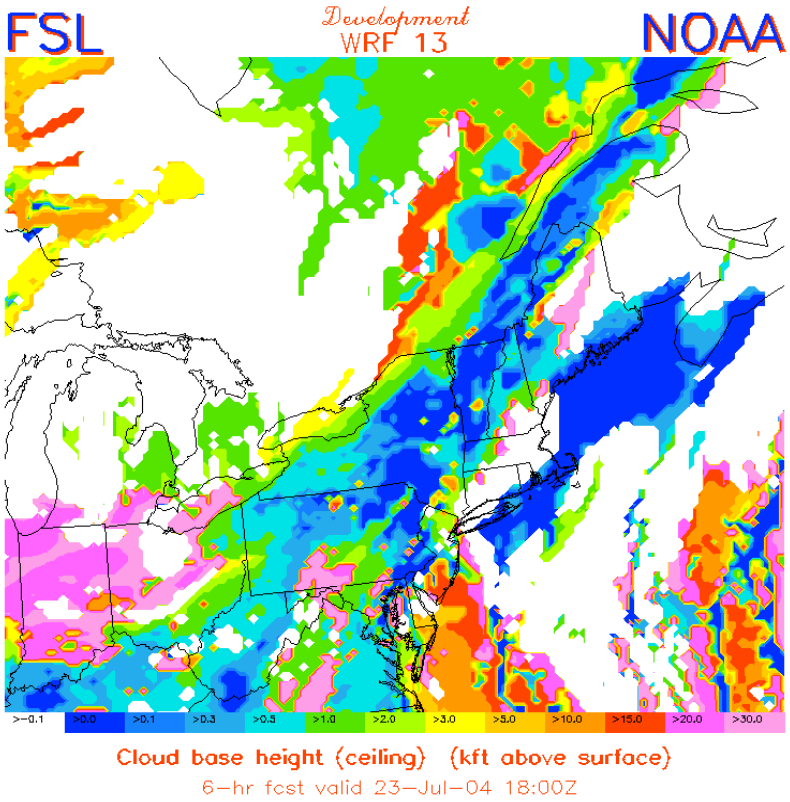
Real-time model verification product:

www.etl.noaa.gov/programs/2004/neaqs/verification

Meteorological Evaluation

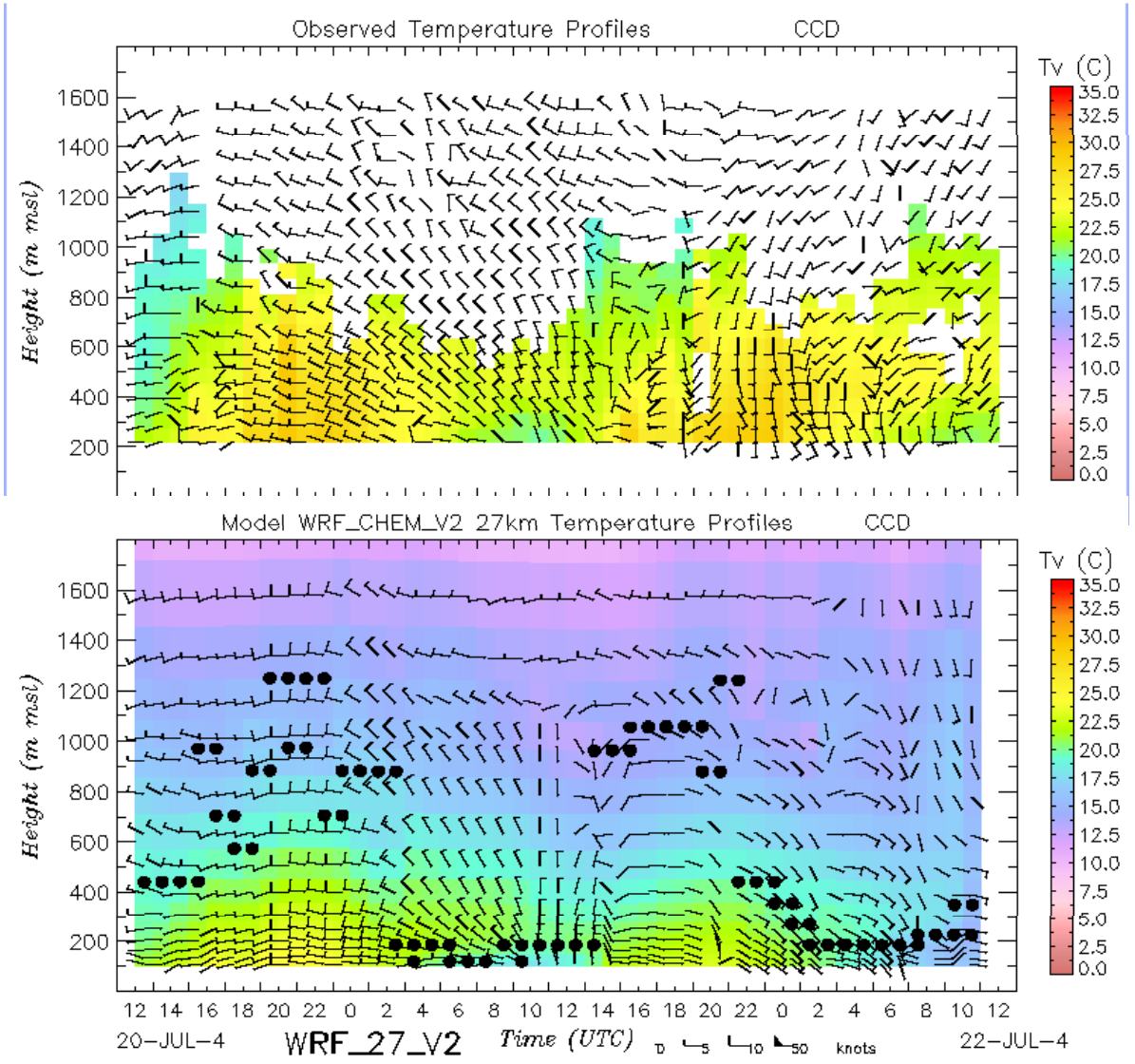
WRF cloud forecasts





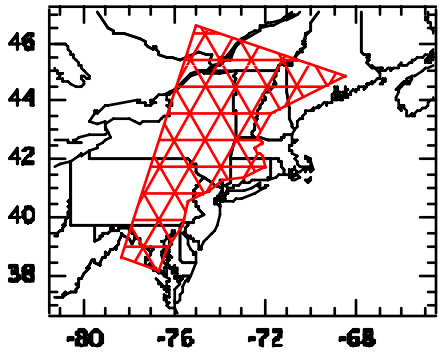
Meteorological Evaluation
LIDAR profile observations vs model forecast at location

- Winds:
  - – Daytime: close
  - –Night: not too good
- Temperature:
  - – MYJ parameterization appears to be too cool
  - – Other PBL paramterizations give different results
  - –Important to initialize soil moisture correctly

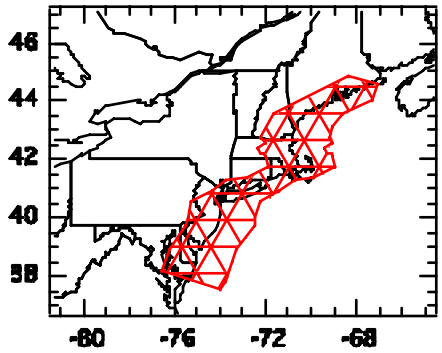


Meteorological evaluation - upper air profiles

Inland Window



Coastal Window



Window data coverage

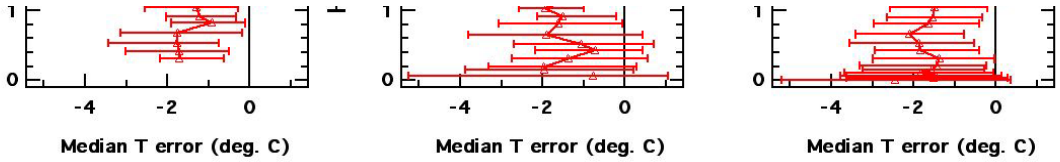
Inland, daytime = 11%

Coastal, daytime =19%

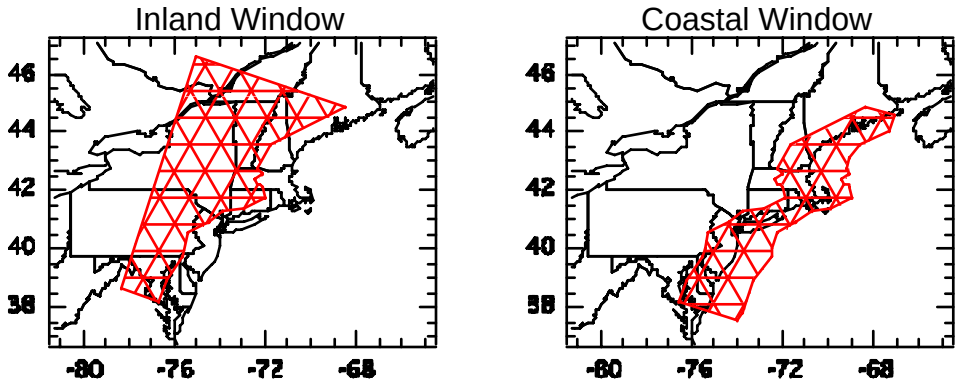
WRF model,
T profiles

Median model error

(MYJ PBL too cool during daytime)



Meteorological evaluation - upper air profiles



Window data coverage

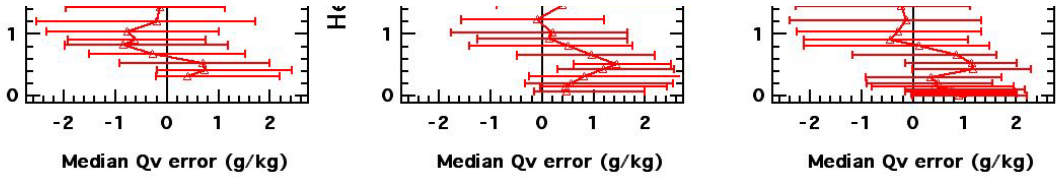
Inland, daytime = 11%

Coastal, daytime =19%

WRF model,
Mixing ratio profiles

Median model error

(MYJ PBL too humid during daytime)

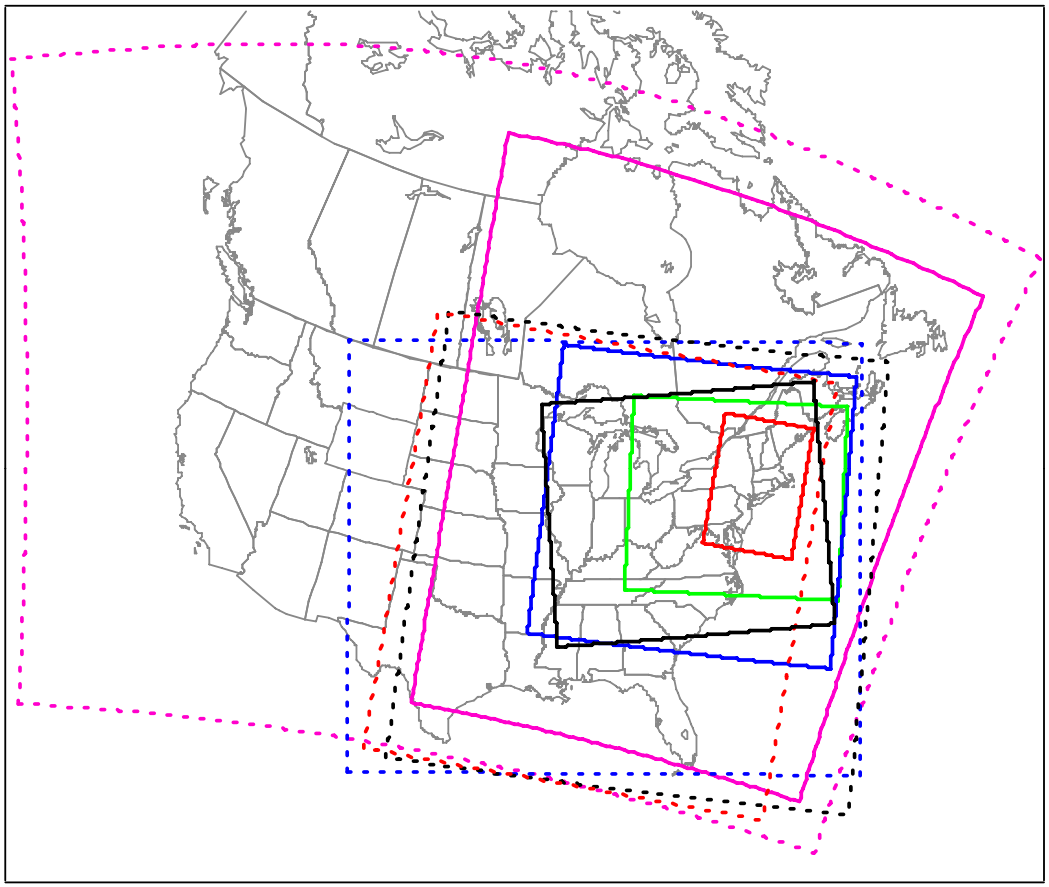


Real-time WRF-Chem

- Statistical Evaluation (Stu McKeen)
  - Surface chemistry observations
  - Tropospheric chemistry observations

TEXAQS 2004

Models Used in the ICARTT/NEAQS-2K4 Evaluations

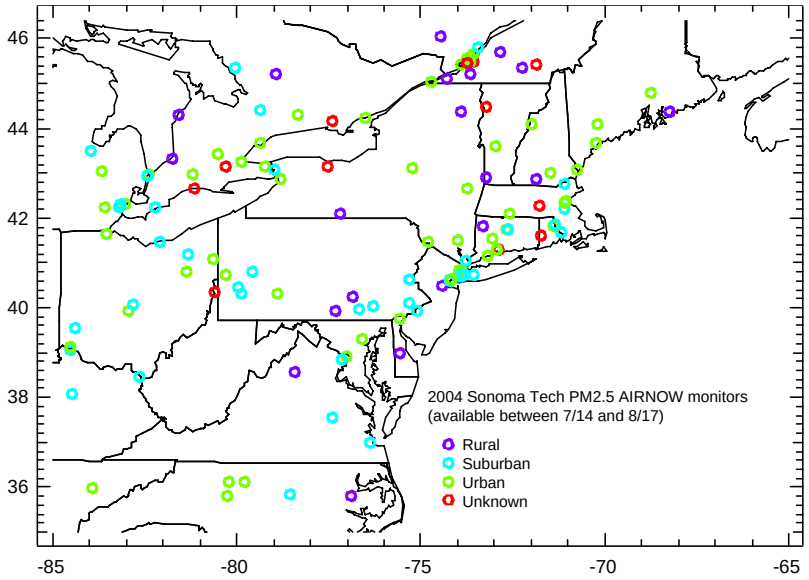


Model:	Anthropogenic Emission Inventory:
AURAMS - 42km CHRONOS - 21km	Canadian National Inv. (1990, 1995)
CMAQ/ETA(1x) - 12km CMAQ/ETA(3x) - 12km(*) BAMS - 45km BAMS - 15km	NEI-99, 2001, grown to 2004
WRF/CHEM-1 - 27km	NEI-96
WRF/CHEM-2 - 27km WRF/CHEM - 12km(*) STEM(2K3) - 12 km	NEI-99

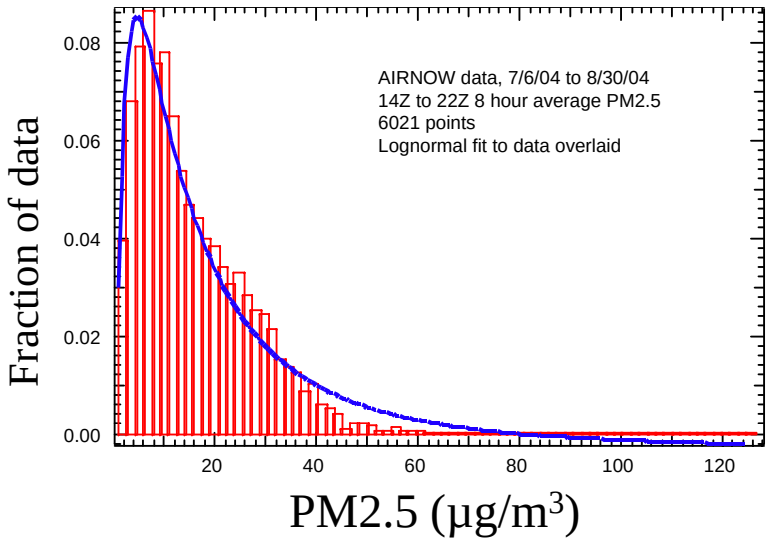
CHRONOS
CMAQ/ETA-3X
WRF/CHM-27km
BAMS -45km
STEM-2K3
AURAMS
CMAQ/ETA-1x
WRF/CHEM-12km
BAMS-15km

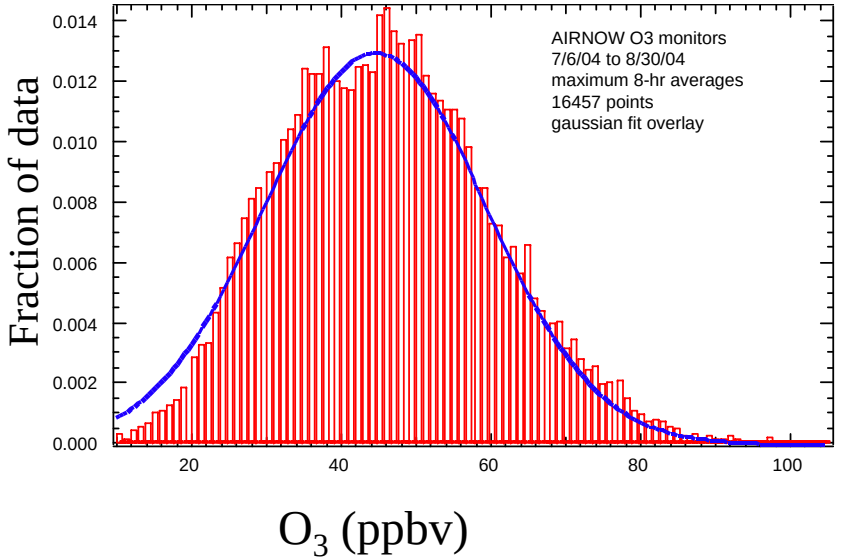
Red indicates PM2.5 forecasts available
(*) Indicates a retrospective run

PM2.5 Monitors - AIRNow network (2004)



- 118 TEOM monitors
- 10 am to 6 pm LDT averages
- No spatial interpolation
- **Log-transformed statistics for PM2.5**
- Only days with complete model overlap
- Only 00Z forecasts analyzed so far





ICARTT/NEAQS-2004: Comparing equivalent PM2.5 and O_3 statistics

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

PM2.5 (log stats)

Statistics for 14Z to 22Z 8-hr averages, based on 00Z forecasts only.
Medians of 118 monitor comparisons

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%

O_3 (linear stats)

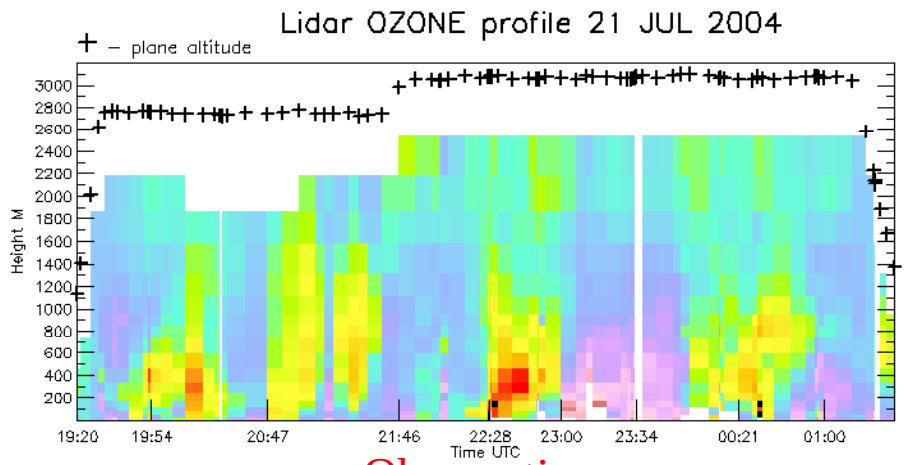
Statistics for maximum 8-hr averages, (00Z forecasts).
Medians of 342 monitor comparisons

r coefficent	Mean bias ppbv	RMSE (ppbv)	Skill (%)
0.67	14.3	20.9	24%
0.73	**3.4**	**11.57**	**61%**
0.68	17.0	23.2	16%
0.54	5.9	16.2	27%
0.60	26.4	31.	2%
0.63	13.4	17.9	24%
0.76	10.2	15.0	47%

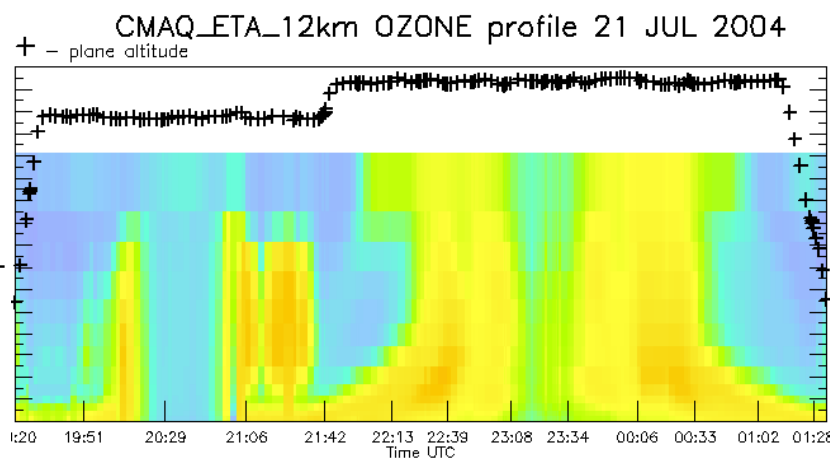
WRF-Chem version 2 improves forecast correlation, reduces ozone bias
- improved emissions, fixed “features” in model

PM2.5 ratio bias near 1! Had expected worse ratio bias

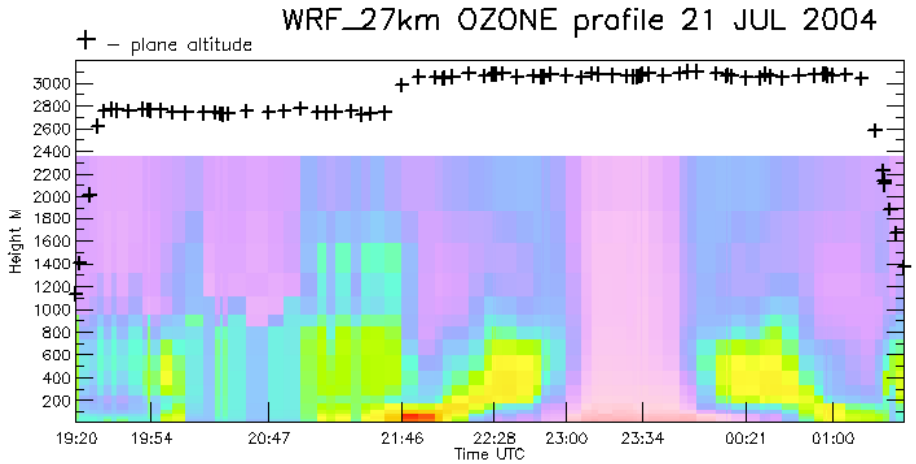
NOAA DC-3 Ozone curtains: observations and model forecasts
July 21, 2004



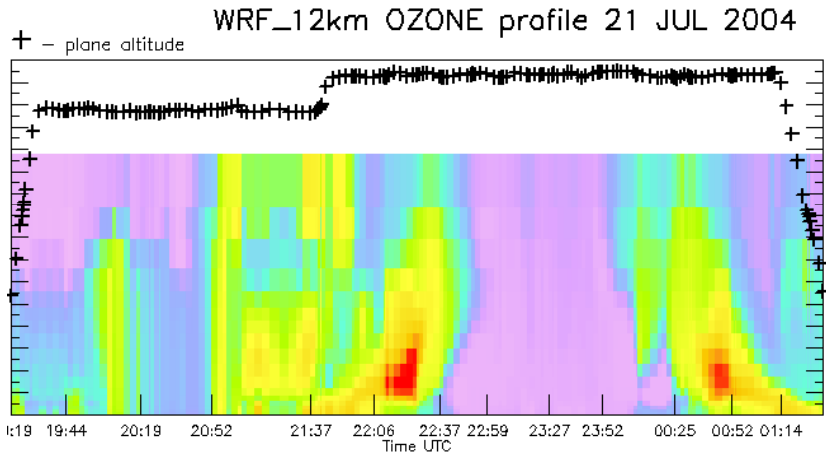
Observations



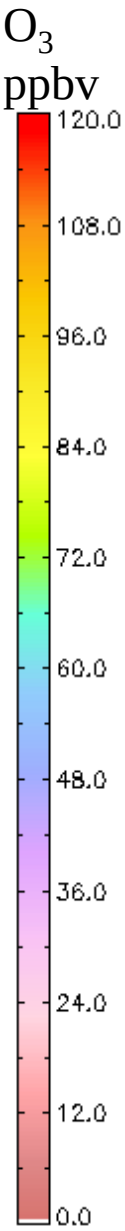
CMAQ/ETA offline Model



WRF-Chem MYJ (2.5) PBL scheme

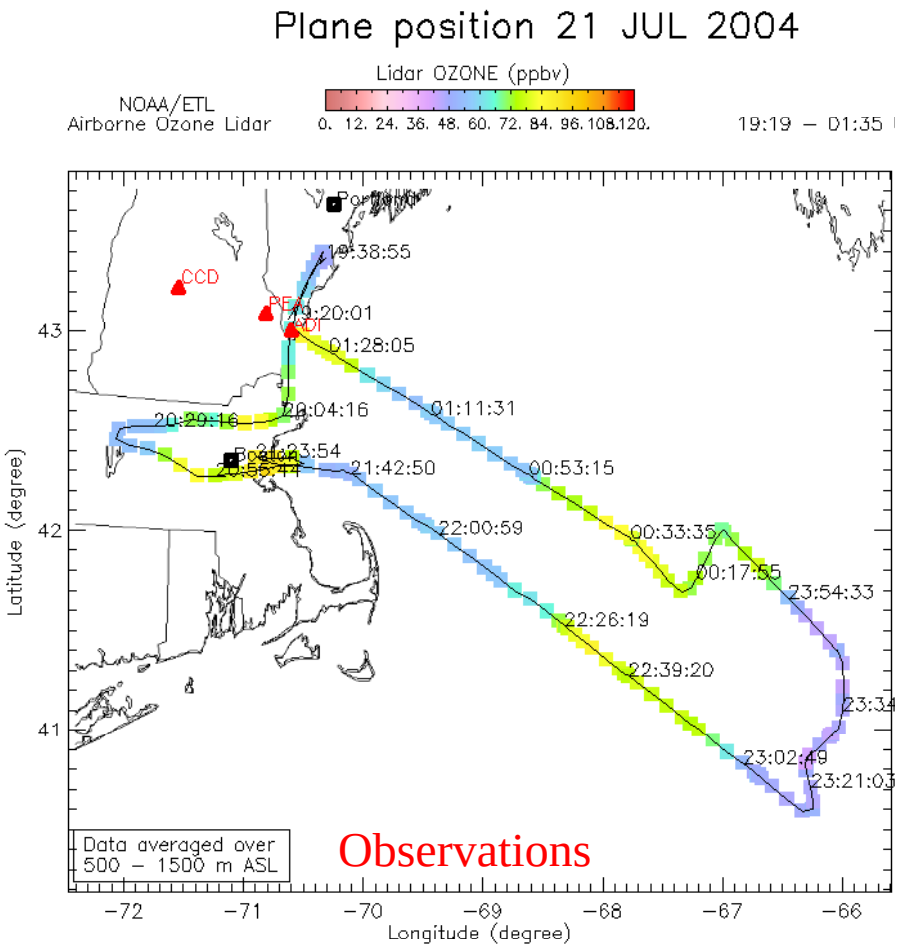


WRF-Chem YSU PBL scheme



NOAA DC-3 Airborne Ozone Lidar

Average PBL Ozone concentration



TEXAQS 2006

Real-time Model Forecasts Collected by CSD during TexAQS-2006
And used within the surface-network and aircraft evaluations:

12km online WRF/Chem (NOAA/GSD) - NEI-99 (March 2004 release)
36km online WRF/Chem (NOAA/GSD) - NEI-99 (March 2004 release)
12km offline CMAQ/WRF-NMM (NCEP) - NEI-2001, Pouliot et al.
21km offline Canadian CHRONOS model (GEMS) - NEI-2001
28km offline Canadian AURAMS model (GEMS) - NEI-2001
5km offline Baron AMS MAQSIP model (MM5) - NEI-2001, Vukovich et al.
15km offline Baron AMS MAQSIP model (MM5) - NEI-2001, Vukovich et al.
20km offline University of Iowa STEM model (MM5, WRF)- NEI-2001, Vukovich et al.

Applications for multi-model evaluations:

Model versus Model Evaluations

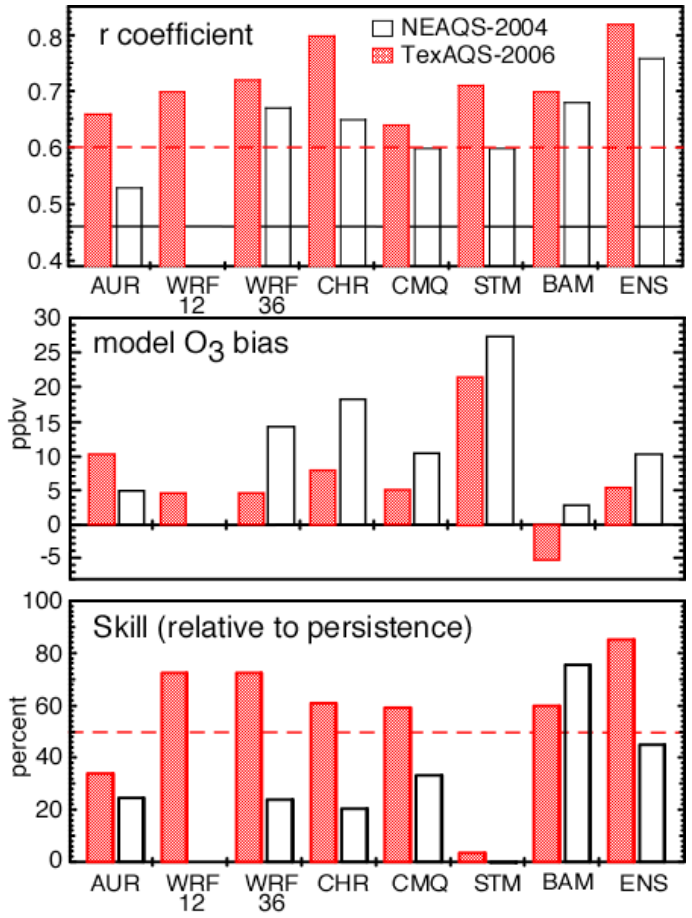
Ensemble Forecasts

Emissions Verification

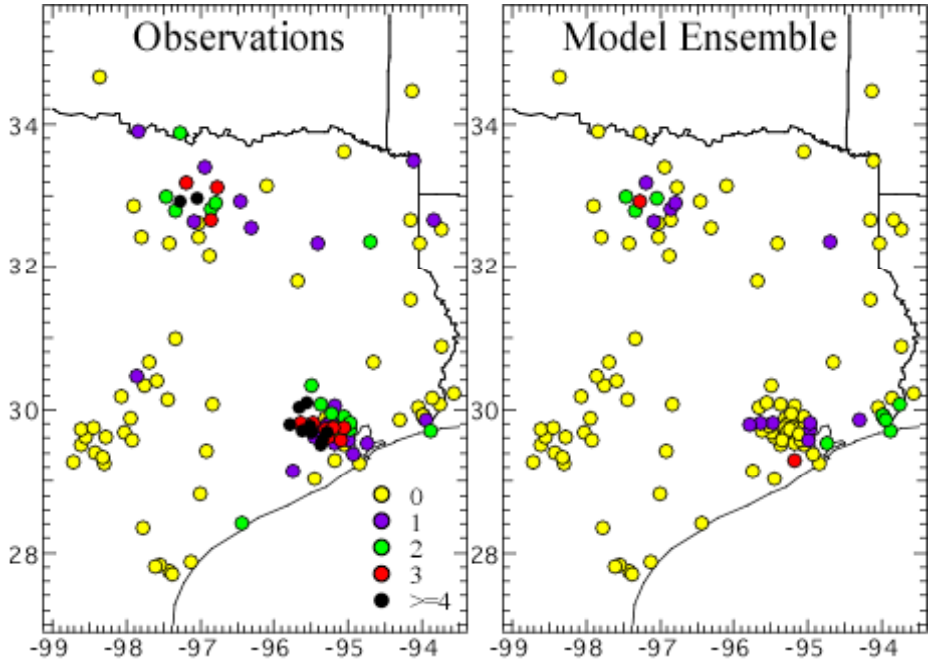
Review: AQ forecast models versus AIRNow surface network

8-hr maximum average O3

Standard Statistics



Number of days 8hr max > 85 ppbv



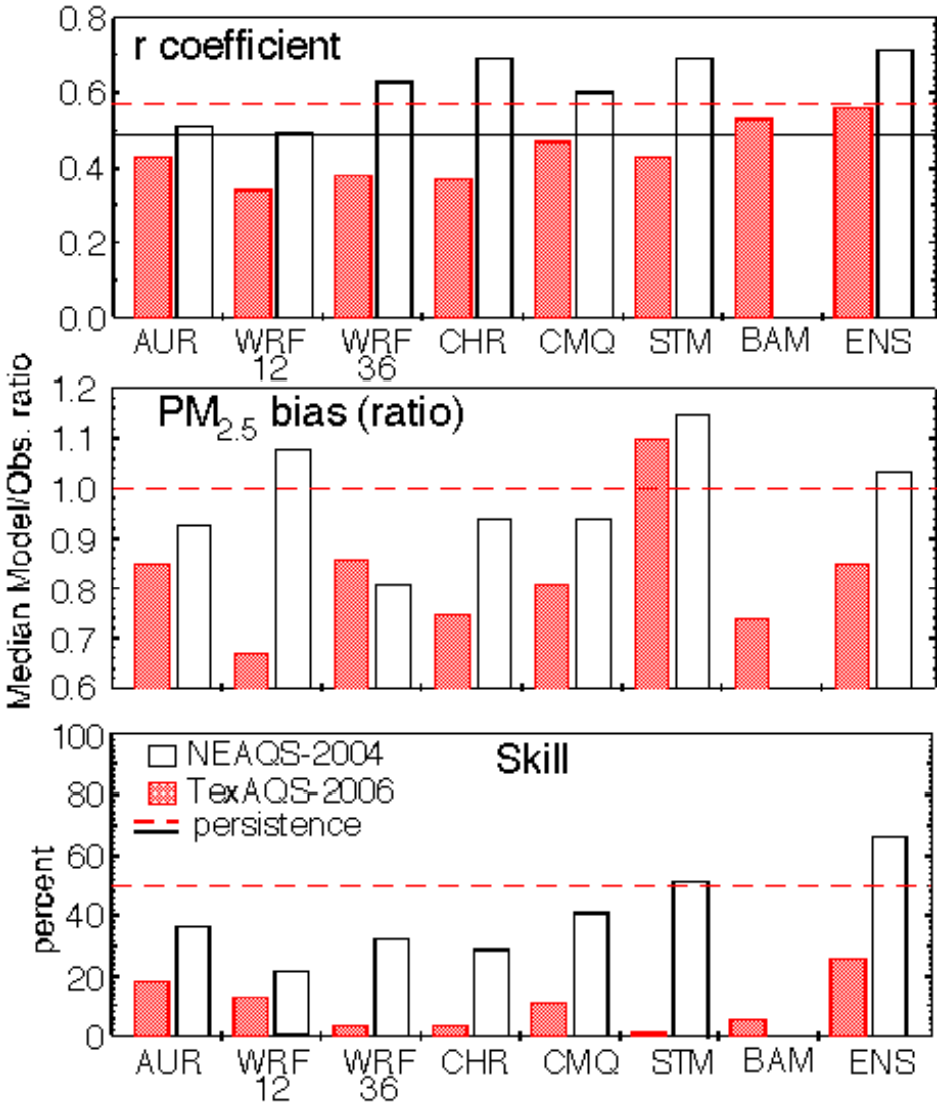
Ensemble of 7 models yields best bulk statistics

TexAQS-2006 forecasts much better than 2004

Number of days > 85 ppbv underpredicted in 2006, particularly in Houston

Review: AQ forecast models versus AIRNow surface network

24-hr avrg.PM2.5



PM2.5 (24-hr) forecasts show less skill than for O3

2006 TexAQS PM2.5 forecasts perform worse than 2004.

Most models biased low (~15%) during TexAQS-2006

The NOAA WP-3D Aircraft Platform during the 2004 and 2006 field studies

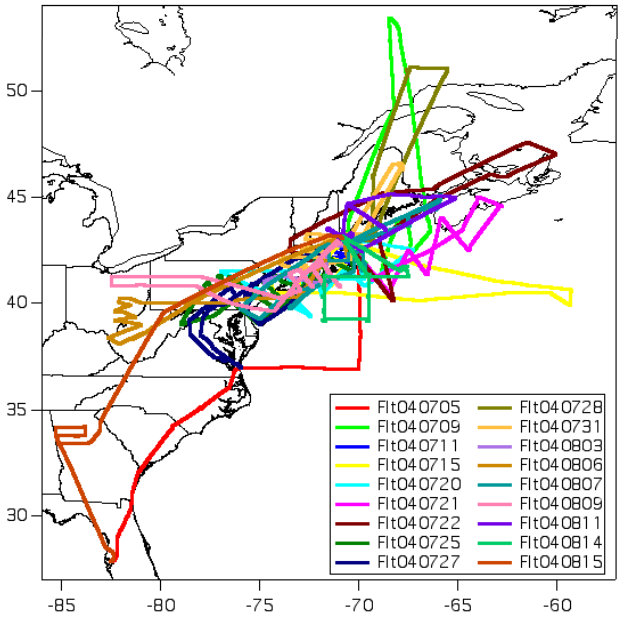
Payload:

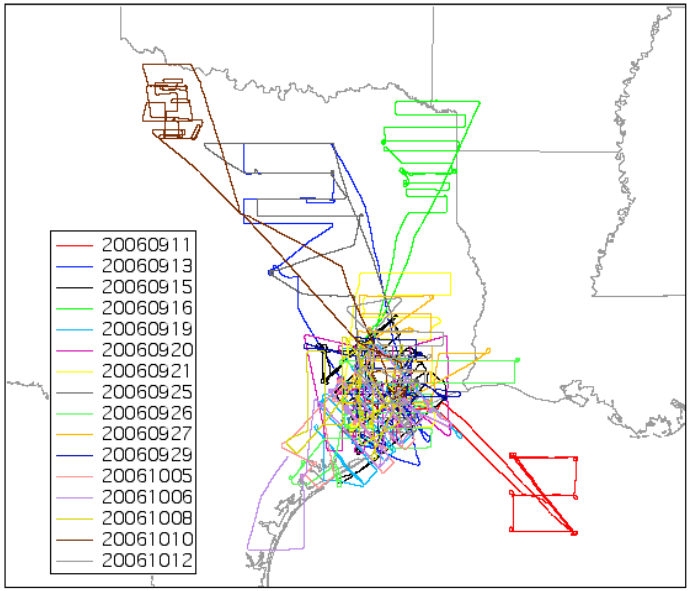
~ 22 gas-phase at (1 to 10 sec res.)
6 PM2.5 constituents
PM2.5 size distributions
Actinic Flux and Radiation
1 second meteorology variables

Flight Patterns:

~ 80% of time 300 and 600 m AGL
0 to 6 km vertical profiles
~ 70% of time from 10am to 4 pm LT
Upwind/Downwind of Urban Plumes

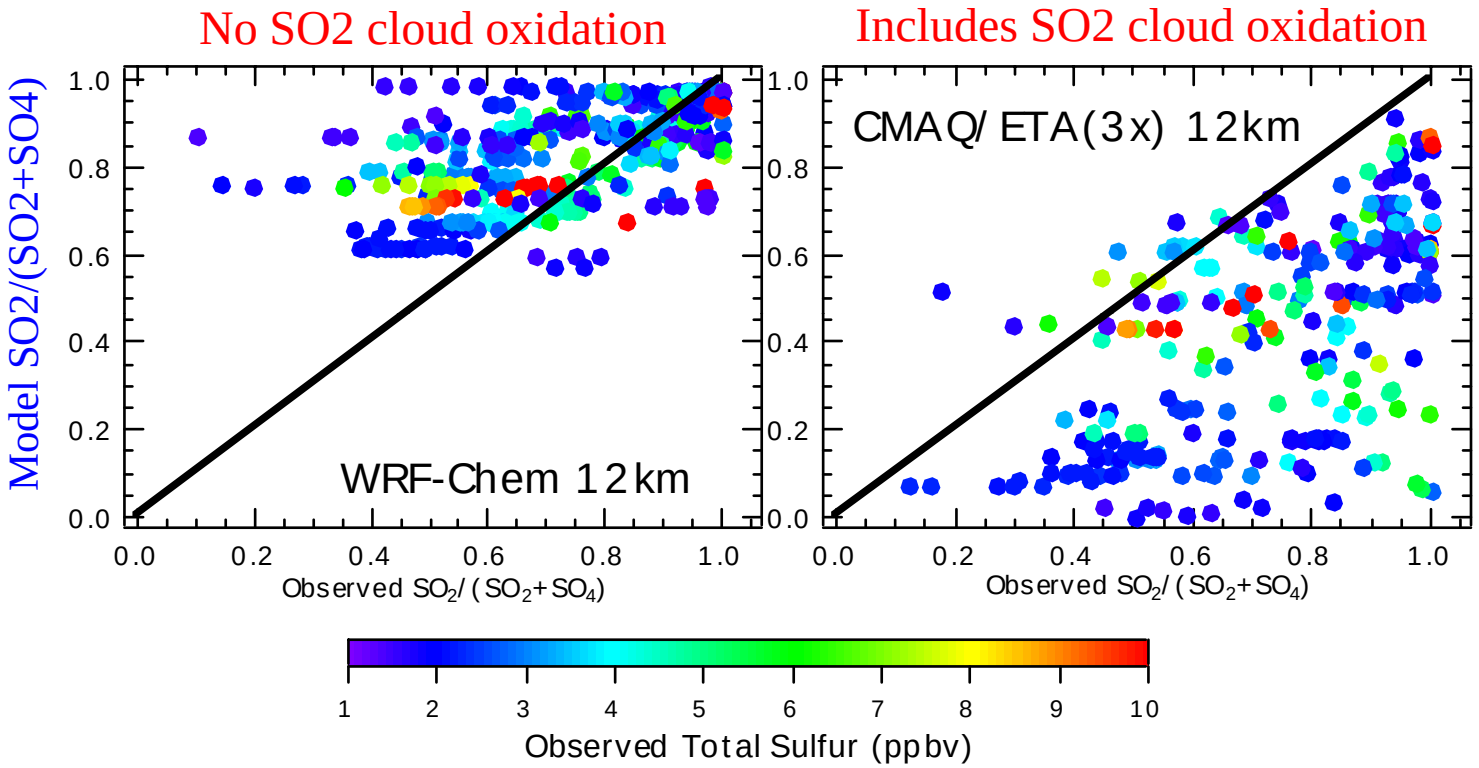
WP-3D evaluation web page:
http://www.esrl.noaa.gov/csd/2006/modeleval/





Comparing SO2 oxidation rates, Models versus Obs.

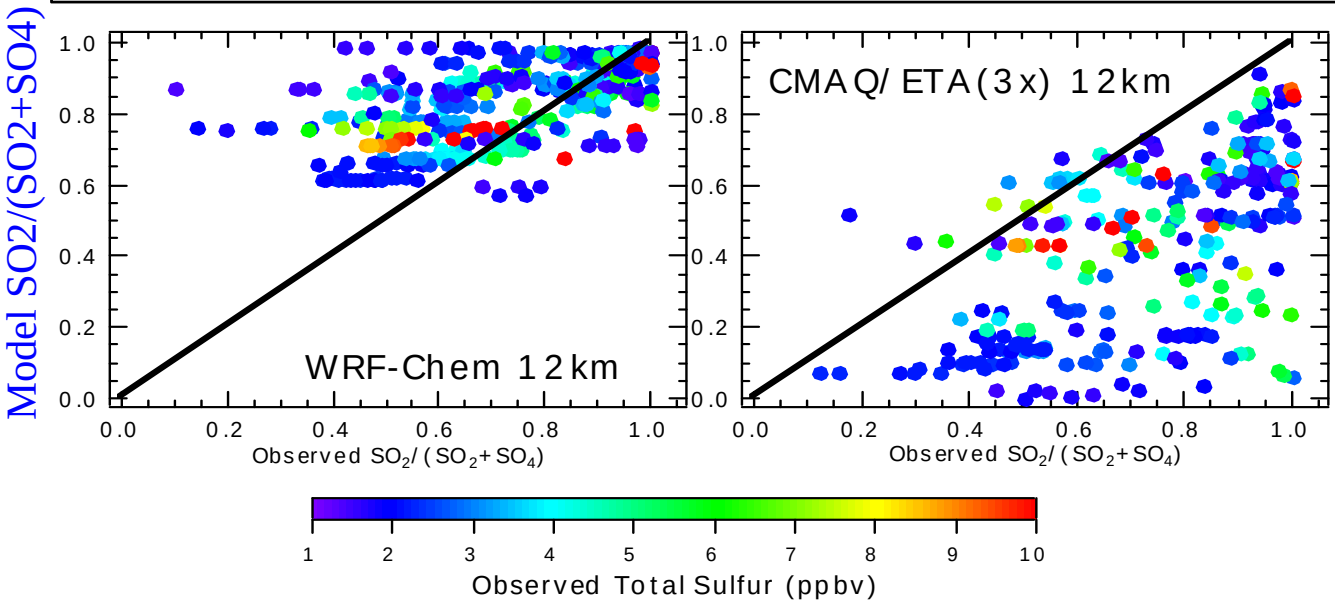
Inland, 410 - 670 meter, 11:00 am to 4:00 pm LT,7 flights 7/15/04 - 7/28/04)

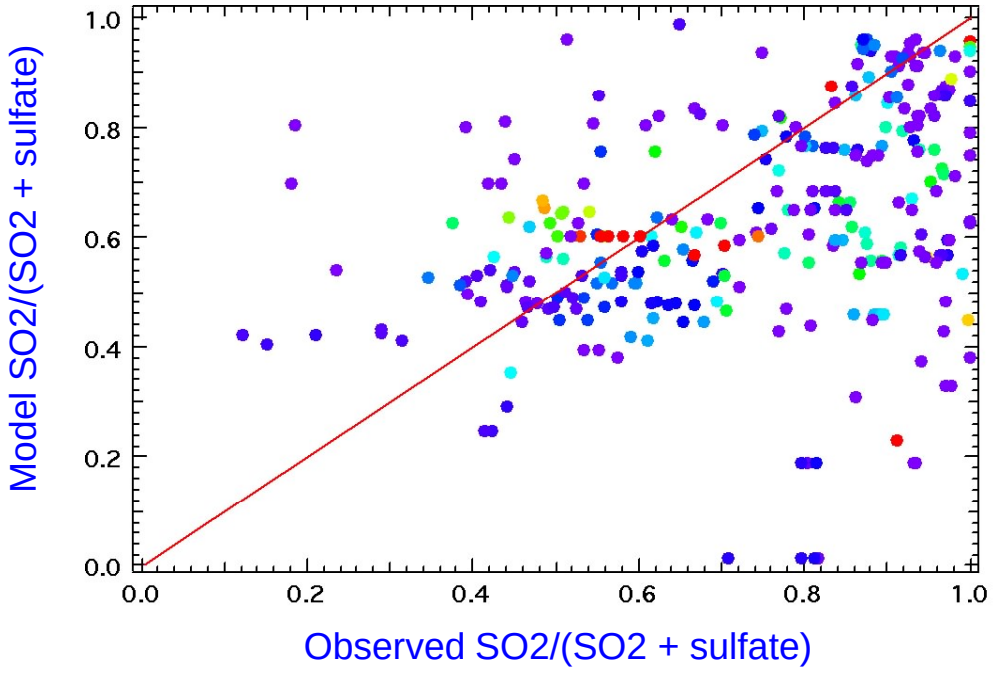


Models without cloud oxidation under-predict SO4 and SO2 oxidation

Models with cloud oxidation over-predict SO4 and SO2 oxidation

WRF/Chem version 3.0 GOCART aerosol - aqueous phase SO2 oxidation

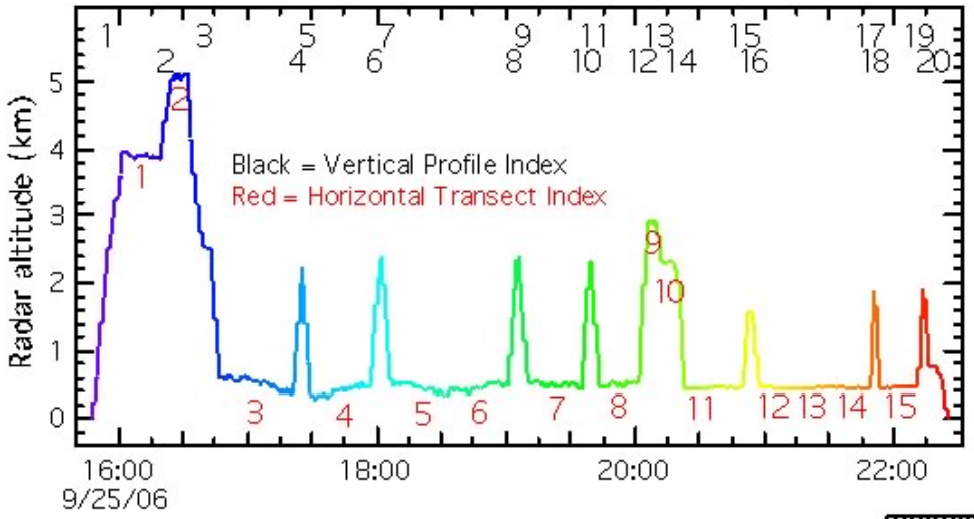


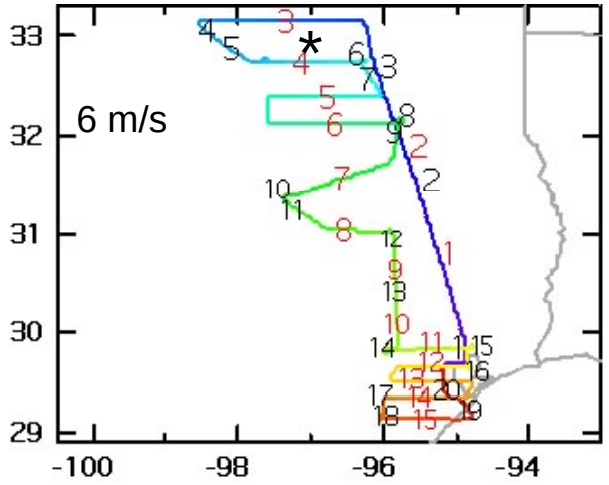


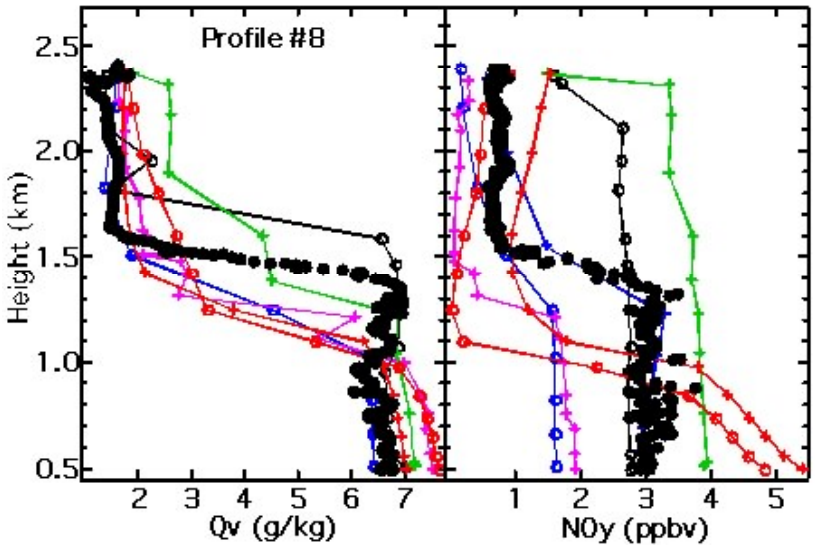
WRF/Chem version 3.0
RACM-GOCART

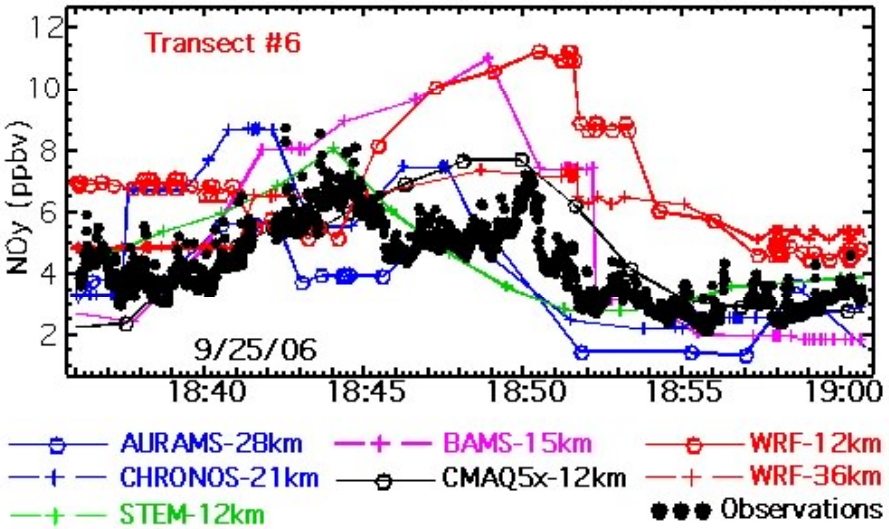
Simple (instantaneous)
Cloud Oxidation of
SO2 with H2O2

TexAQS-2006, Upwind and Downwind Sampling of Houston and Dallas
(Example of 9/25/06 flight, transect 80 km downwind of Dallas)



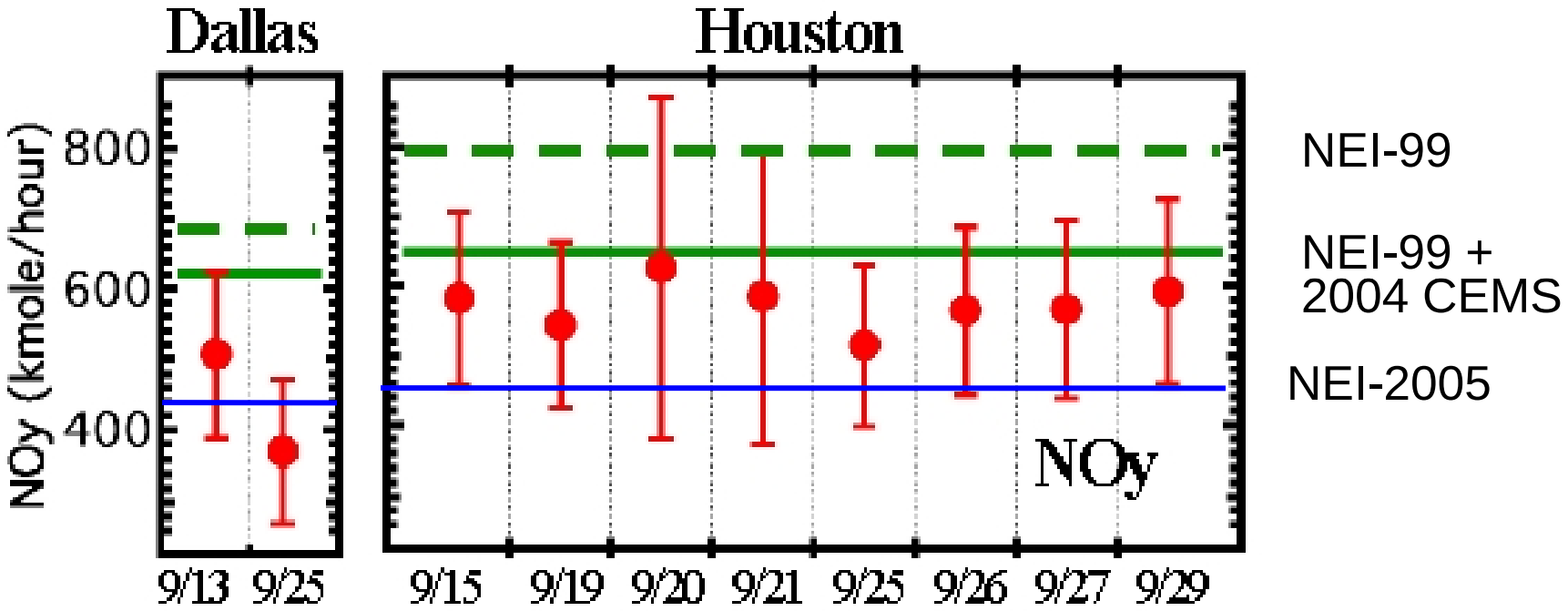






Observed and Inventory Emission Estimates of NOy for Dallas and Houston:

NOy 11:00 am LT emissions from Houston and Dallas
Derived from upwind/downwind transects, and emission inventories

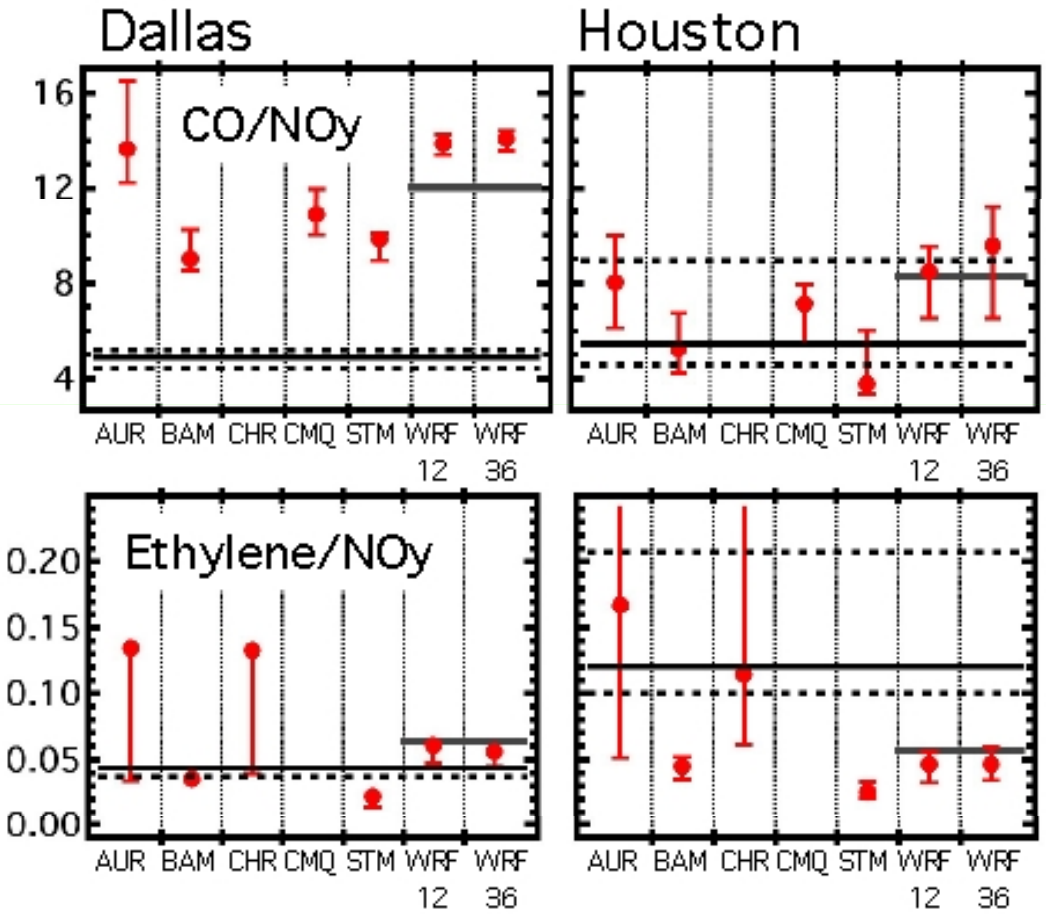


Uncertainty limits in observations include PBL and background uncertainties

Emission inventory from 11:00am to noon, LT (representative of daylight average)

over pre-determined ~1000 km_2 domains

Model and Observed concentration difference ratios (and NEI-99 emission ratios) downwind (< 50 km) of Houston and Dallas



Concentration difference ratios reproduce emission ratios

Dallas CO/NOy high by a factor of 2 for all models

Canadian Models:
Ethylene from biogenic sources

Houston Ethylene/NOy low by a factor of 2 for other models

Red circles: Model median ratios (whiskers - central 2/3 of sorted distributions)

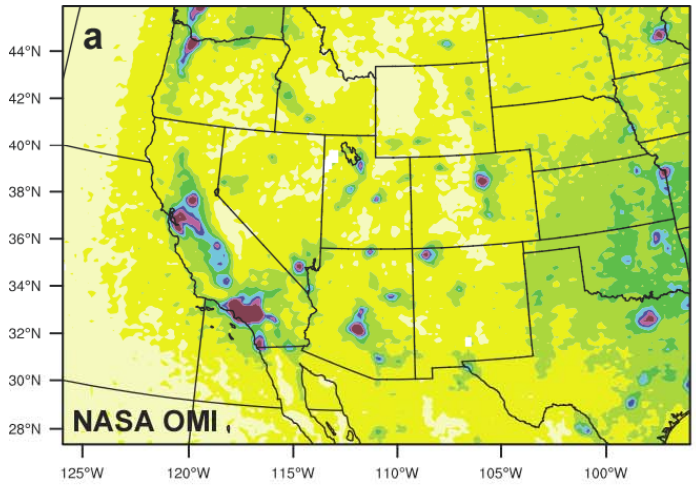
Black lines: Observed medians (dashed lines - central 2/3 of sorted distributions)

Gray lines over WRF/Chem models - From NEI-99 (used in WRF/Chem runs)

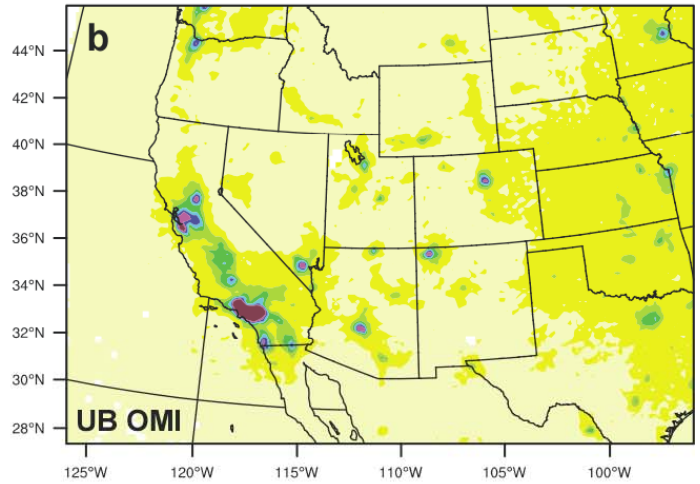
OMI satellite NO column comparisons

Summer of 2005 averages, 10:30 Local Time overpass

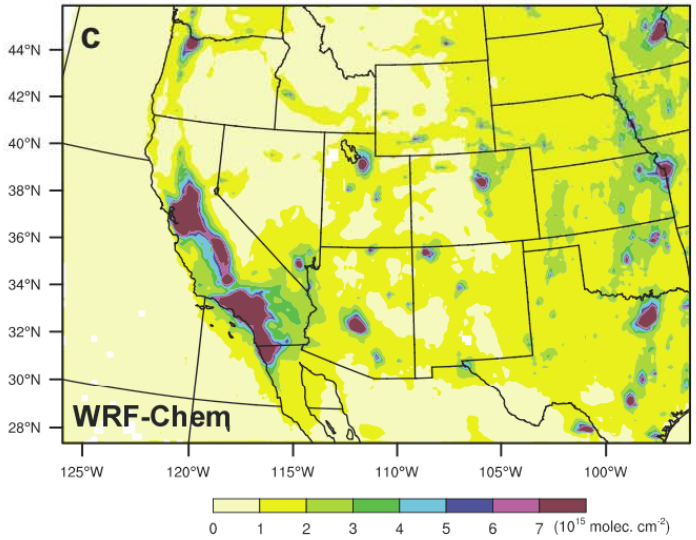
NASA retrieval



University of Bremen retrieval



WRF/Chem model



Current real time

– a new domain

– a new grid spacing

– a new set of problems?

Real Time AQ Forecasts

http://ruc.noaa.gov/hrrr

Every 6 h over the western US (as of Aug08)

Real-time fire information (GOES ABBA) to provide air quality guidance

Uses radar-enhanced RUC-DFI (Digital Filter Initialization) grids

- atmospheric initial conditions, same as hourly NE Corridor HRRR.

Cycled chemistry variables, including:

- Ozone,
- PM 10 aerosol,
- PM 2.5 aerosol.

Includes direct effect feedback from atmospheric aerosols

Real Time AQ Forecast Domain

HRRRchem domain:

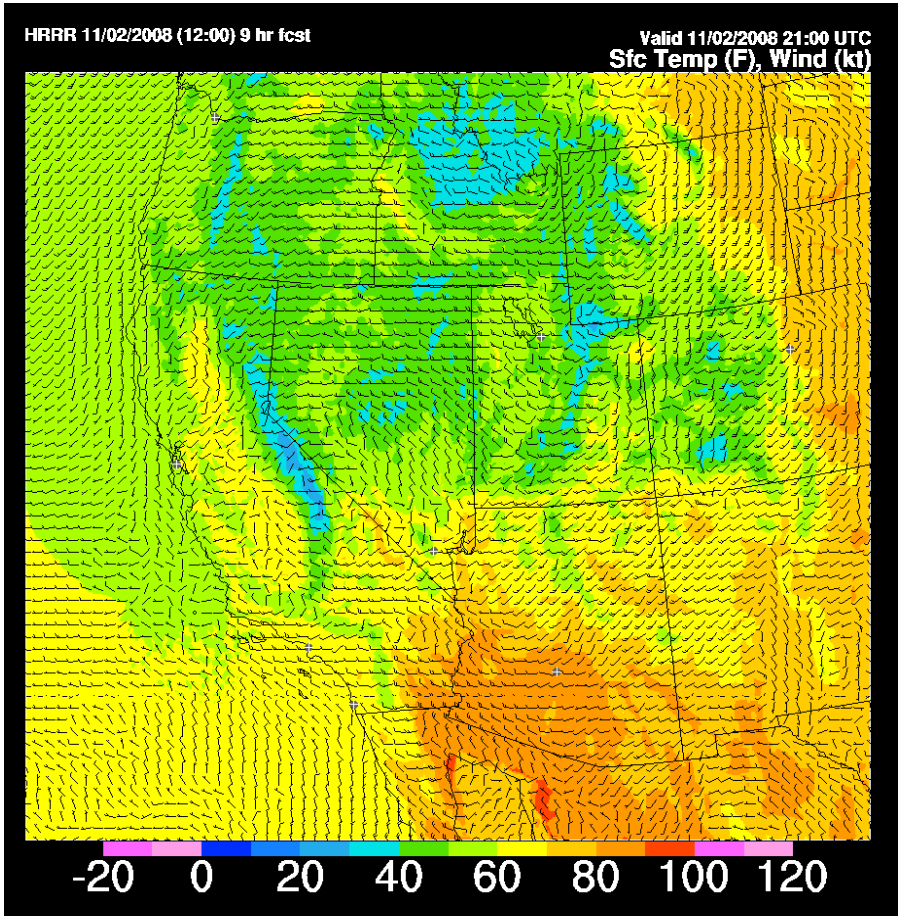
- 3 km horizontal grid
- 711 x 647 grid points
- 51 Vertical levels
  - Vertical stretched

Physics options:

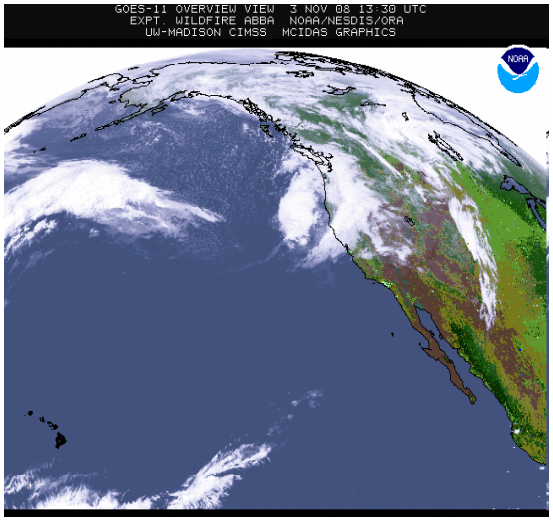
- Thompson microphysics
- Goddard SW
- RRTM LW scheme
- RUC land surface
- MYJ TKE PBL scheme

Chemistry options:

- RADM2/SORGAM
- Aerosol-Radiation feedback (direct effect)



Real Time AQ Forecast: Wild Fire location



http://cimss.ssec.wisc.edu/goes/burn/wfabba.html

Wildfire Automated Biomass Burning Algorithm (WFABBA)

- half-hourly fire data for the Western Hemisphere.
  - GOES-11 covers North America only.
  - GOES-12 provides coverage for North and South America

Images available online as well.

- WFABBA imagery is generated using a modified alpha-blending technique.
- Data from GOES and a landcover map derived from 1-km resolution Advanced Very High Resolution Radiometer (AVHRR)

Real Time AQ Forecast: Wild Fire location

Run prep-chem-sources to get wild fire locations onto model domain

Combine files from past 1.5 days to remove cloudy sky issues

Files containing WF-ABBA data on /public/data/sat

f20082900000.namer.v61.g11.filt
f20082900030.namer.v61.g11.filt
f20082900100.namer.v61.g11.filt

Format (ASCII with header)*

NOAA/NESDIS/ORA University of Wisconsin-Madison/CIMSS
GOES-11 WF_ABBA (vs 6.1) Experimental Filtered Fire Product
Note: This product is preliminary and has not been quality controlled
Date: 2008290 Time: 0 UTC Filtered file: 12 hours 24 files

Longitude	Latitude	T4(K)	T11(K)	Size(km2)	Temp(K)	Ecosystem	Fire Flag
-124.74	55.21	299.9	273.2	-9.0000	-9.	21	3
-123.54	54.73	317.5	275.0	-9.0000	-9.	21	3
-123.56	54.65	307.1	275.0	-9.0000	-9.	21	5
-116.41	47.22	294.6	264.4	-9.0000	-9.	22	3
-116.74	46.81	290.8	260.4	-9.0000	-9.	22	3
-115.89	46.47	299.8	277.4	-9.0000	-9.	20	3
-119.67	37.56	304.0	291.0	-9.0000	-9.	22	2

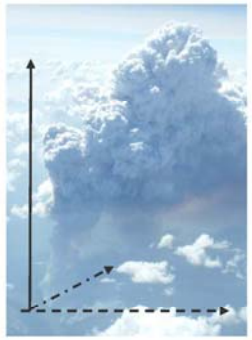
* Mainly use first two columns

Real Time AQ Forecast: Fire emissions

Including fire emissions in the model

Biomass burning and wildfires

Smoldering : mostly surface emission.
Flaming: mostly direct injection in the PBL, free troposphere or stratosphere.

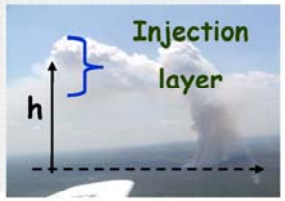


Plume rise model

total emission flux: F_η being λ the smoldering fraction

smoldering term : $E_\eta = \dfrac{\lambda F_\eta}{\rho_{air} \Delta z_{\text{first phys. model layer}}}$

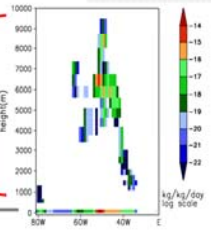
flaming term : $E_\eta = \dfrac{(1-\lambda) F_\eta}{\rho_{air} \Delta z_{\text{injection layer}}}$

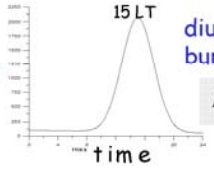


Example in the model:

flaming emission

smoldering emission



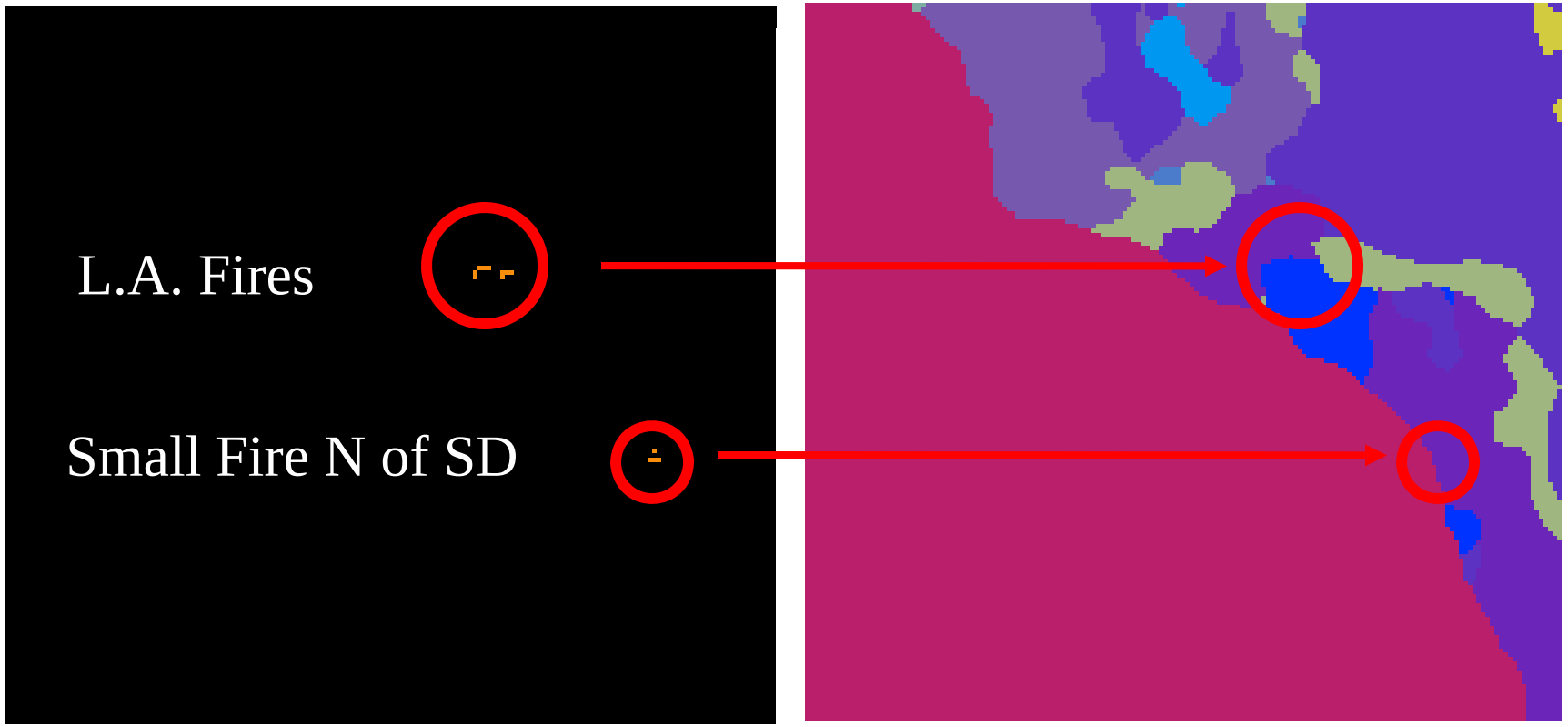


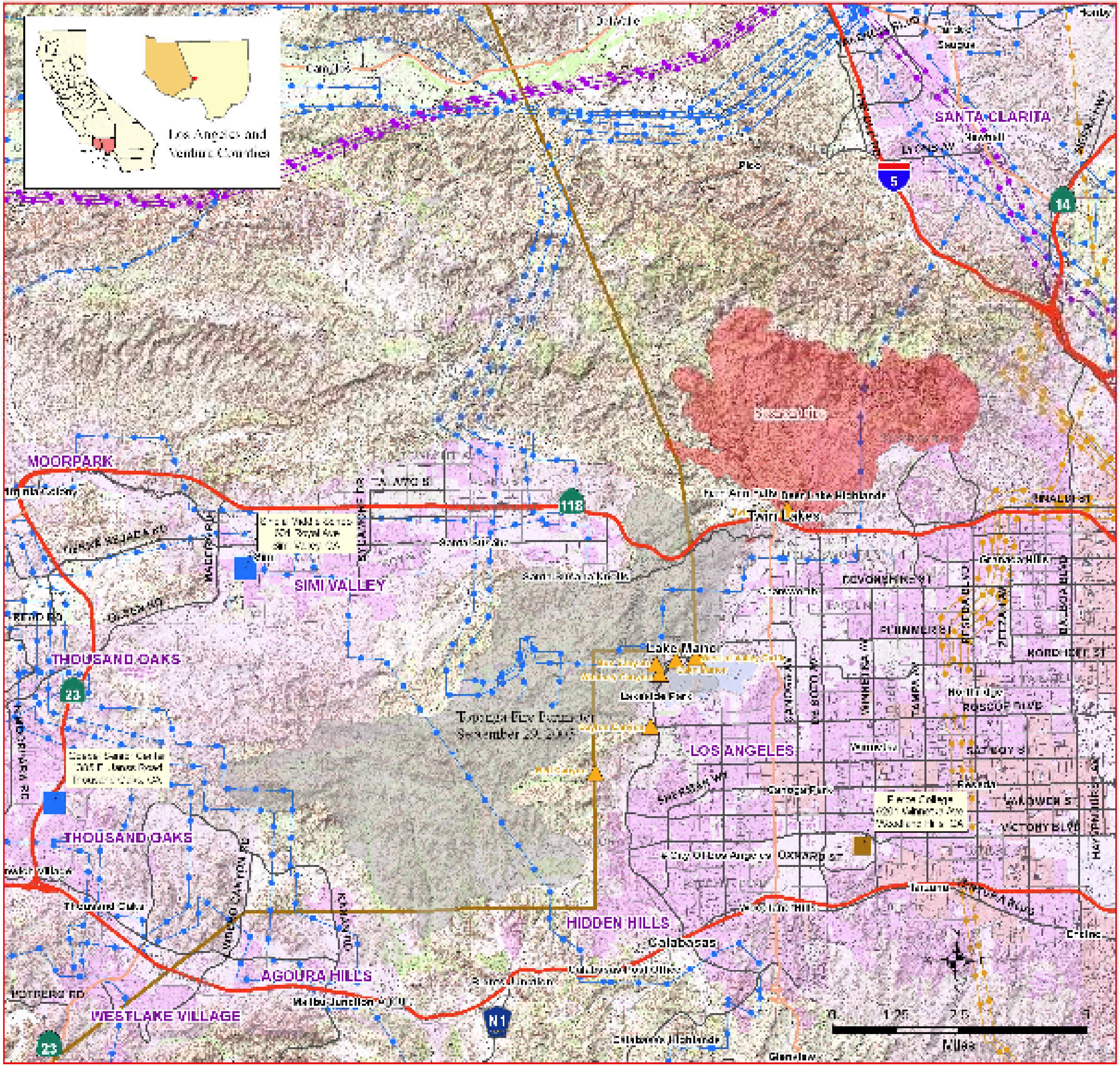
$r(t)$

diurnal cycle of the burning for S. America:

$E_\eta(t) = r(t) E_\eta$

Real Time AQ Forecast: Wild Fire location





SESNON FIRE

CA-LAC-08216155
as of 10/14/08 - 0700 Hrs
9,872 Acres 0% Contained
Started October 13, 2008 1058 Hrs
Los Angeles/Ventura Counties
FMAG Approved #2789

Fire Threats and Damages:
19 Residences Destroyed
3,500 Residences Threatened
100 Commercial Properties Threatened

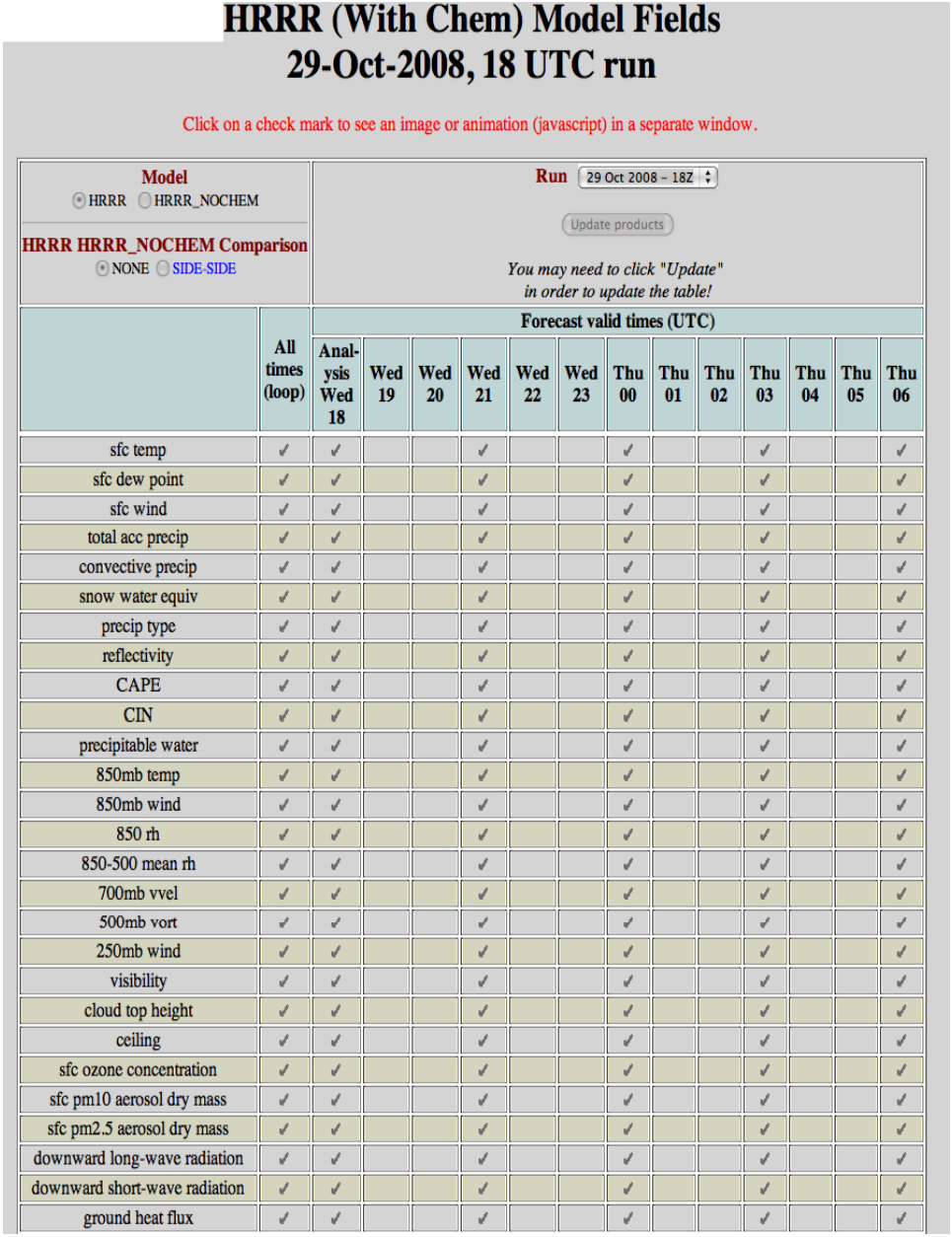
[illegible]

Fire Perimeter as of 10/13/08 - 2100 Hrs
Evacuation Sites 10/13/08
Evacuation Center
Domestic Animal Shelter
Evacuated Canyons
Major Roads (TBM)
Freeway
Highway
Primary
Secondary
Transmission Line
SCE - 66KV
SCE - 220KV
LADWP - 230KV
Topanga Fire Perimeter as of 9/28/05
Incorporated City Limits

HRRR-Chem products available online

http://www-frd.fsl.noaa.gov/mab/hrrr3wchem/

Comparison with HRRR forecast not using chemistry



HRRR (With Chem) Model Fields
29-Oct-2008, 18 UTC run

Click on a check mark to see an image or animation (javascript) in a separate window.

Model
(•) HRRR ( ) HRRR_NOCHEM

HRRR HRRR_NOCHEM Comparison
(•) NONE ( ) SIDE-SIDE

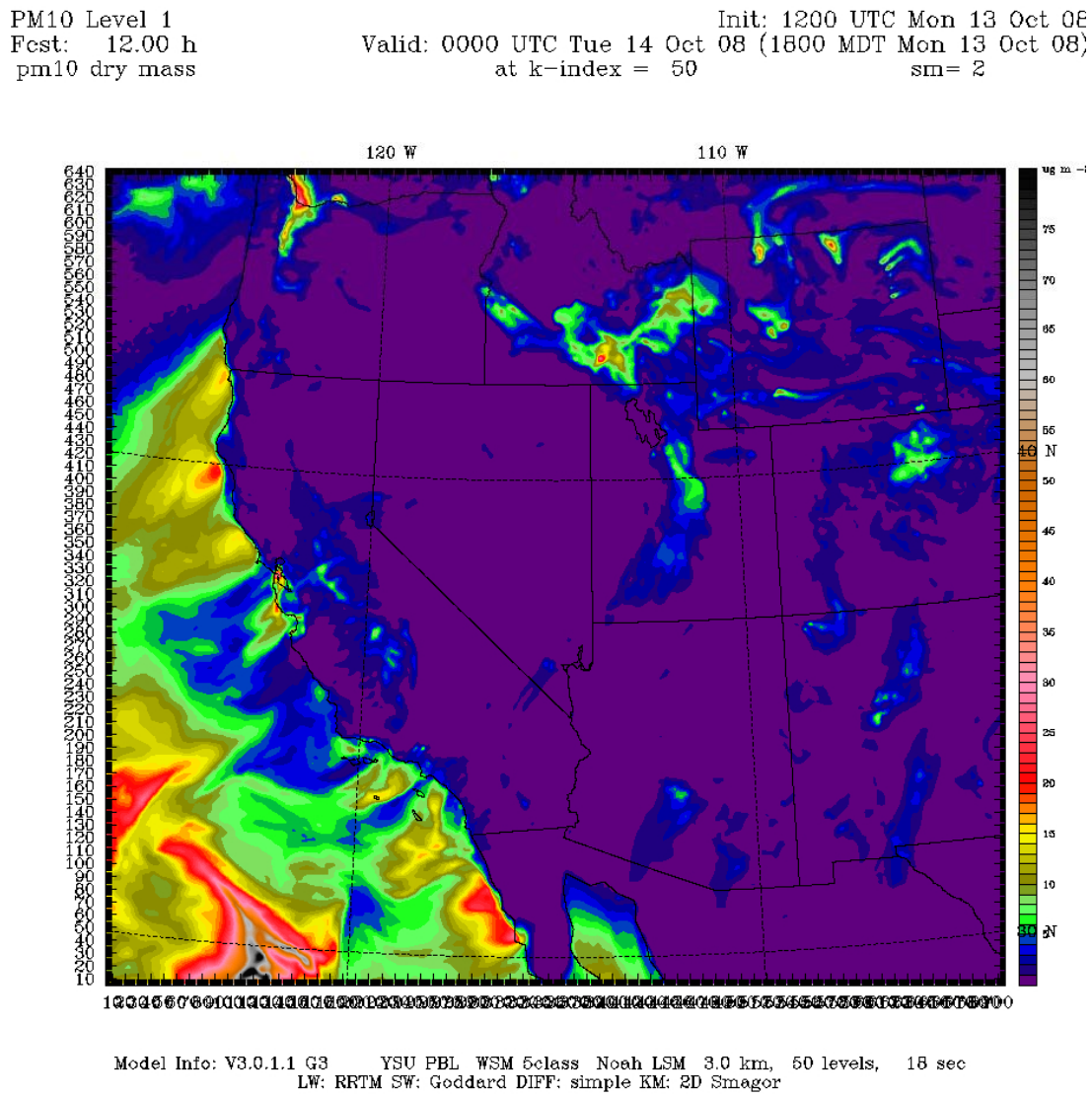
Run 29 Oct 2008 - 18Z

Update products

You may need to click "Update" in order to update the table!

	All times (loop)	Forecast valid times (UTC)												
		Anal-ysis Wed 18	Wed 19	Wed 20	Wed 21	Wed 22	Wed 23	Thu 00	Thu 01	Thu 02	Thu 03	Thu 04	Thu 05	Thu 06
sfc temp	✓	✓			✓			✓			✓			✓
sfc dew point	✓	✓			✓			✓			✓			✓
sfc wind	✓	✓			✓			✓			✓			✓
total acc precip	✓	✓			✓			✓			✓			✓
convective precip	✓	✓			✓			✓			✓			✓
snow water equiv	✓	✓			✓			✓			✓			✓
precip type	✓	✓			✓			✓			✓			✓
reflectivity	✓	✓			✓			✓			✓			✓
CAPE	✓	✓			✓			✓			✓			✓
CIN	✓	✓			✓			✓			✓			✓
precipitable water	✓	✓			✓			✓			✓			✓
850mb temp	✓	✓			✓			✓			✓			✓
850mb wind	✓	✓			✓			✓			✓			✓
850 rh	✓	✓			✓			✓			✓			✓
850-500 mean rh	✓	✓			✓			✓			✓			✓
700mb vvel	✓	✓			✓			✓			✓			✓
500mb vort	✓	✓			✓			✓			✓			✓
250mb wind	✓	✓			✓			✓			✓			✓
visibility	✓	✓			✓			✓			✓			✓
cloud top height	✓	✓			✓			✓			✓			✓
ceiling	✓	✓			✓			✓			✓			✓
sfc ozone concentration	✓	✓			✓			✓			✓			✓
sfc pm10 aerosol dry mass	✓	✓			✓			✓			✓			✓
sfc pm2.5 aerosol dry mass	✓	✓			✓			✓			✓			✓
downward long-wave radiation	✓	✓			✓			✓			✓			✓
downward short-wave radiation	✓	✓			✓			✓			✓			✓
ground heat flux	✓	✓			✓			✓			✓			✓

Real Time AQ Forecast



Summary

- WRF-Chem can be used for real-time forecasts
  - The model is not too complex
  - Shows improvement over time (typical for any model)
- Graphical products can be made available in real-time through a variety of methods
  - Use of web is an idea pathway to end user
  - Need to know your customer and provide products designed to their need
    - Do not need to provide every data array

Summary

- Making the forecast is not the end of the process as evaluation needs to take place
  - Need to examine model data and compare with available observations
    - Ideally evaluations conducted by others
    - Meteorology
    - Chemistry
  - Need to demonstrate “three-dimensional thinking” whenever possible
    - Surface data provides only part of the answer
    - Different model parameter choices can produce very different results
      - User should carefully examine the choices and be aware of the impact of their selections
    - There is no single perfect numerical model
      - Ensemble techniques show great promise

Summary

Chemistry evaluation - look at the whole picture (surface and upper air)
- evaluate model and current scientific understanding

- WRF/Chem O3 photochemistry conforms to available observations
- WRF/Chem (and other models) PM2.5 less reliable sensitive to several processes with large uncertainties
- Simple GOcart Aerosol Option shows marked improvement in simulating aqueous-phase SO2 conversion
- Chemistry biases very sensitive to PBL scheme
- Emissions (both from inventories and satellite data) are changing rapidly
- 2005 NEI NOy emissions consistent with 2006 observations (+/- 25%)
- Developed a technique to relate raw model output to emission ratios:
  - High CO/NOy ratios for all models (but little effect on O3)
  - Ethylene/NOy consistent for Dallas, too low for Houston
- Satellite comparisons useful in emissions verification and satellite retrieval validation