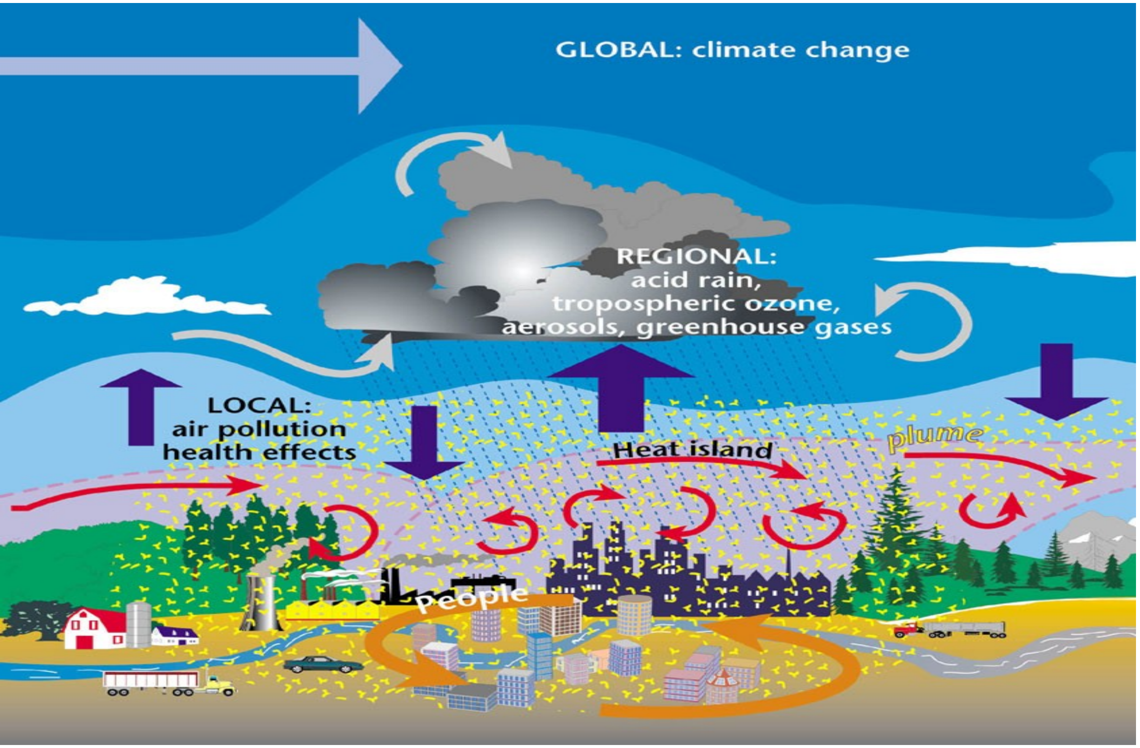
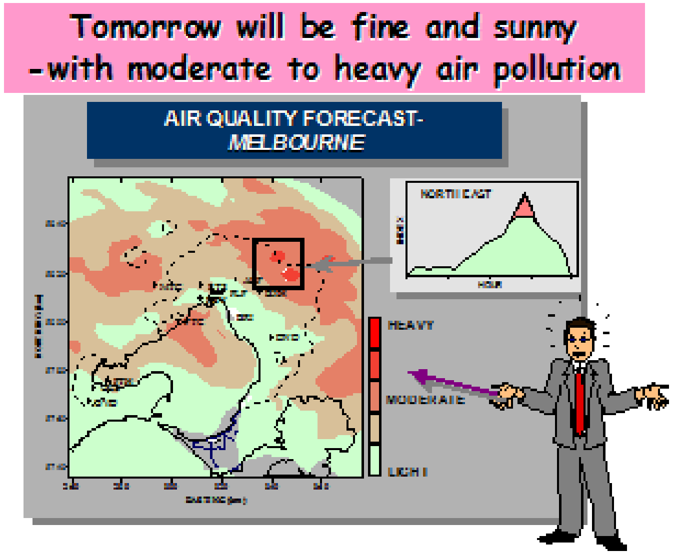
Chemical Weather – A New Challenge/Opportunity For Weather And Other Services

Evolving complexity of observing systems, models, and applications.

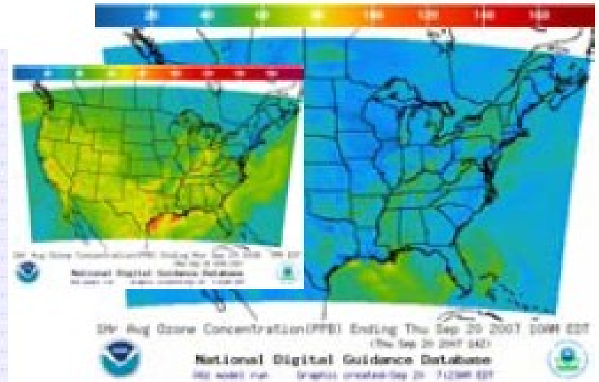


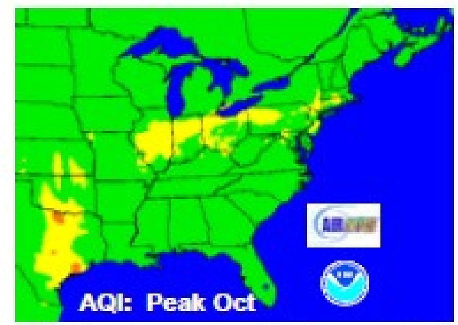


What air quality services can and should be provided?

WMO: GAW Urban Research Meteorology and Environment Project -- GURME

Air Quality Forecast Capability
End-to-End Operational Capability





Model Components: Linked numerical prediction system

Operationally integrated on NCEP's supercomputer

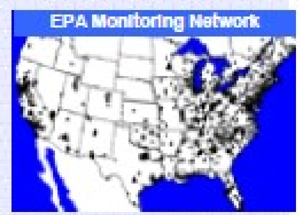
- *NCEP mesoscale NWP: WRF-NMM*
- *NOAA/EPA community model for AQ: CMAQ*

Observational Input:

- *NWS weather observations; NESDIS fire locations*
- *EPA emissions inventory*

Gridded forecast guidance products

- *On NWS servers: www.weather.gov/aq and ftp-servers*
- *On EPA servers*
- *Updated 2x daily*



Verification basis, near-real time:

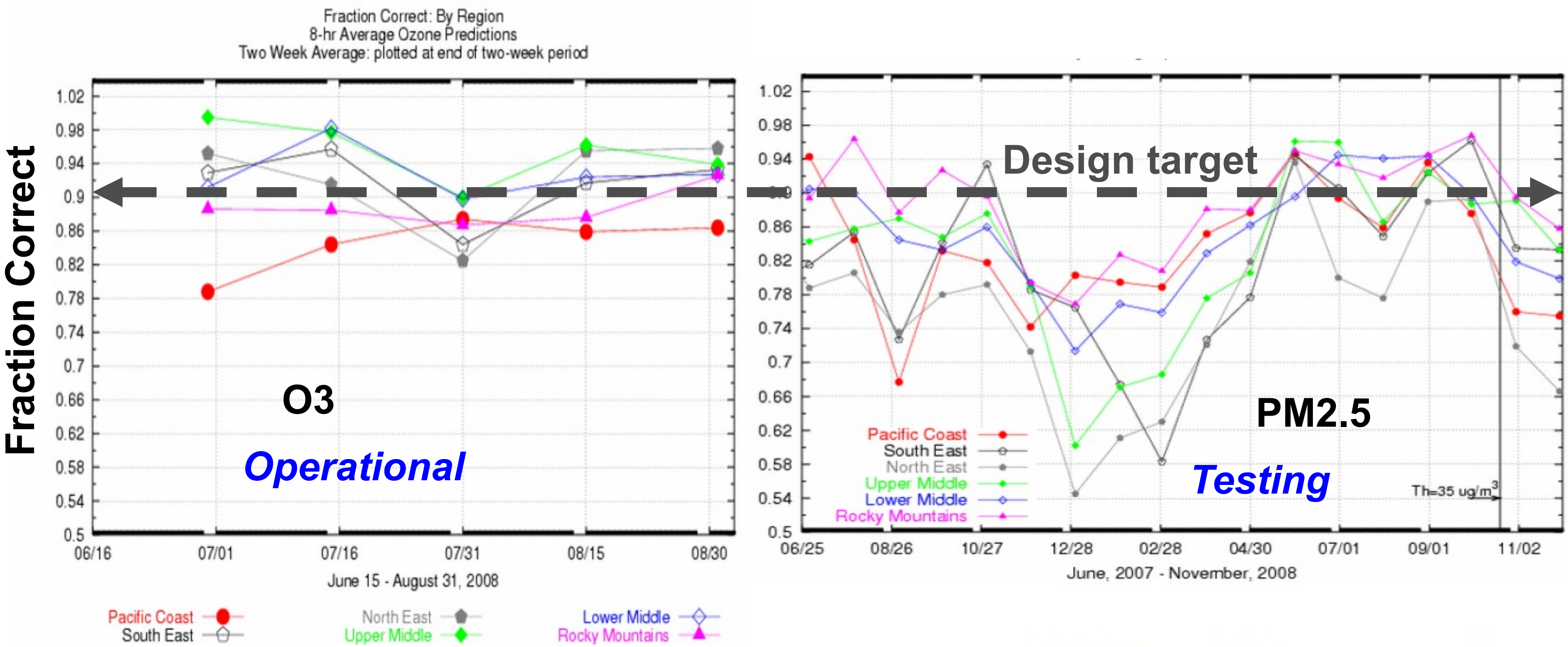
- *Ground-level AIRNow observations*
- *Satellite smoke observations*

Customer outreach/feedback

- *State & Local AQ forecasters coordinated with EPA*
- *Public and Private Sector AQ constituents*
- *Website monitoring*

Slide provided by Paula Davidson

Forecast Skill By Region Of NOAA's Ozone And PM2.5 Predictions

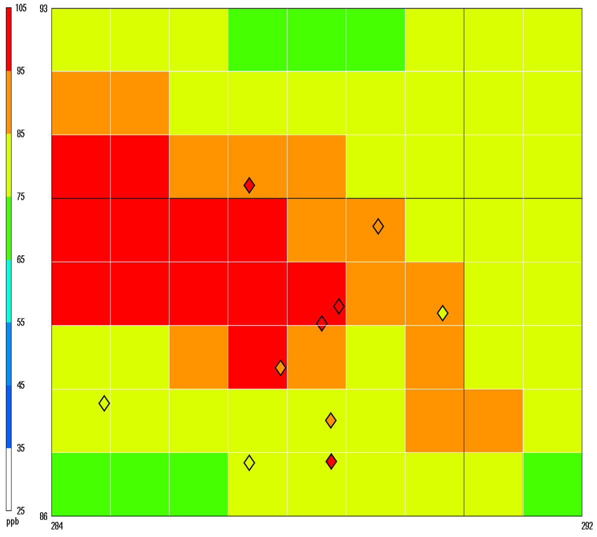


Slide provided by Paula Davidson

Evaluation

Discrete Forecast / Evaluation

Observed *vs.* Forecast Max. 8 hr. Concentration



Example of strict grid-cell to monitor matching

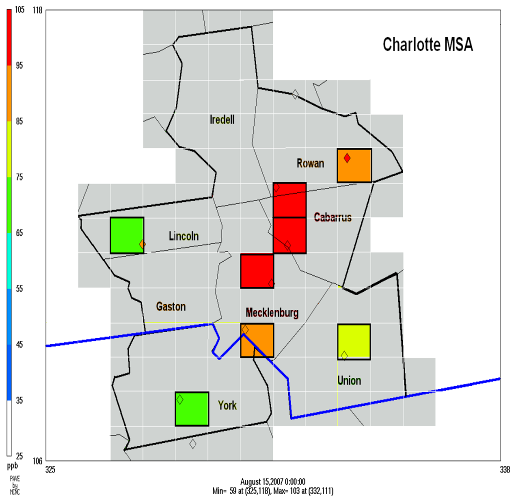
CONUS Forecasts for the Summer (J, J, A)

	n	OBS (ppb)	MOD (ppb)	RMSE (ppb)	NME (%)	MB (ppb)	NMB (%)	r
2007	99132	49.0	53.2	13.0	20.4	4.2	8.7	0.70
2008	99343	47.6	51.6	12.6	20.3	4.0	8.4	0.67

Eder et al., 2009

Current Evaluation Approach

The statistics below are based on using all 8 monitors in the Charlotte MSA with the ***monitors matched directly with their grid cell.***

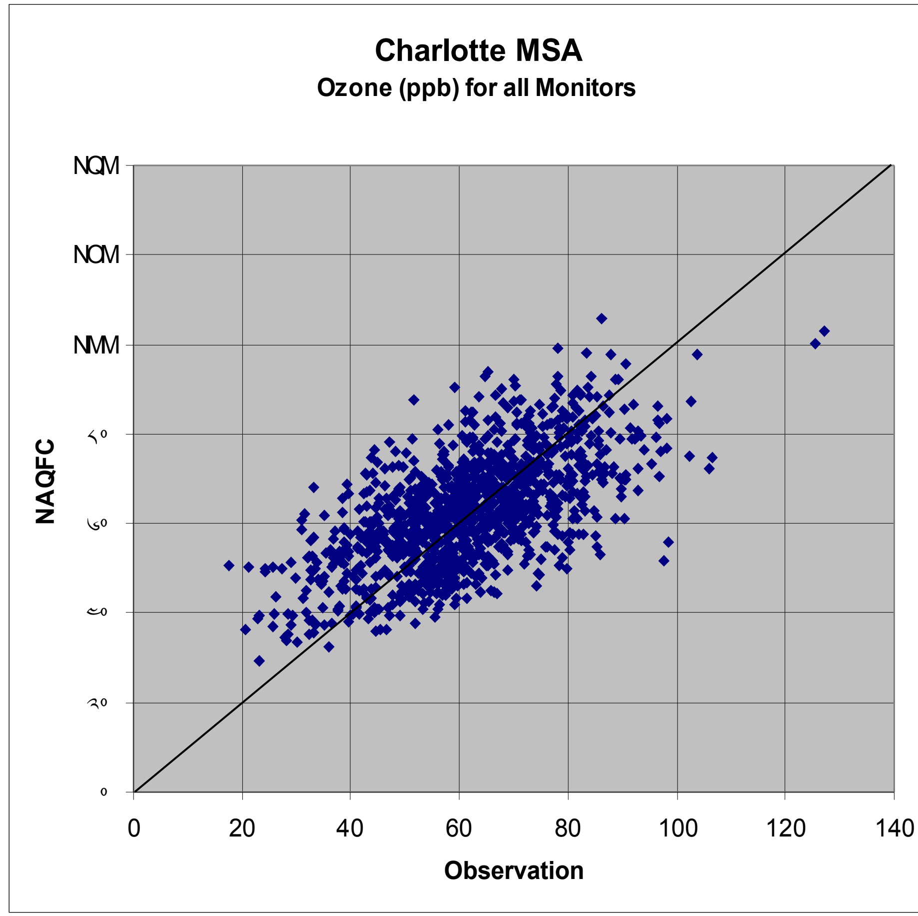


Period: 1 May – 30 Sept. 2007
n = 1207

MB = 2.1 ppb; NMB = 3.3%

RMSE = 12.0 ppb; NME = 16.8%

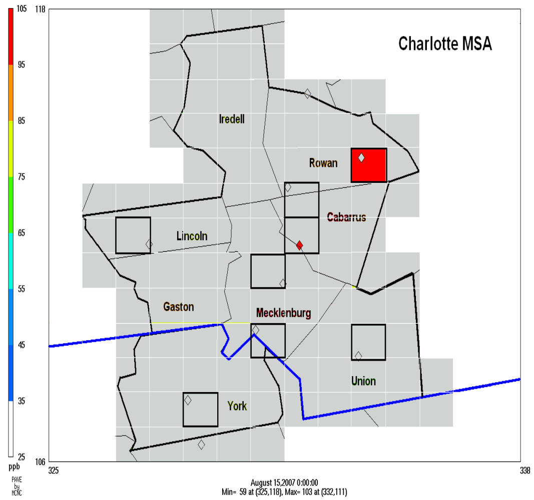
r = 0.63

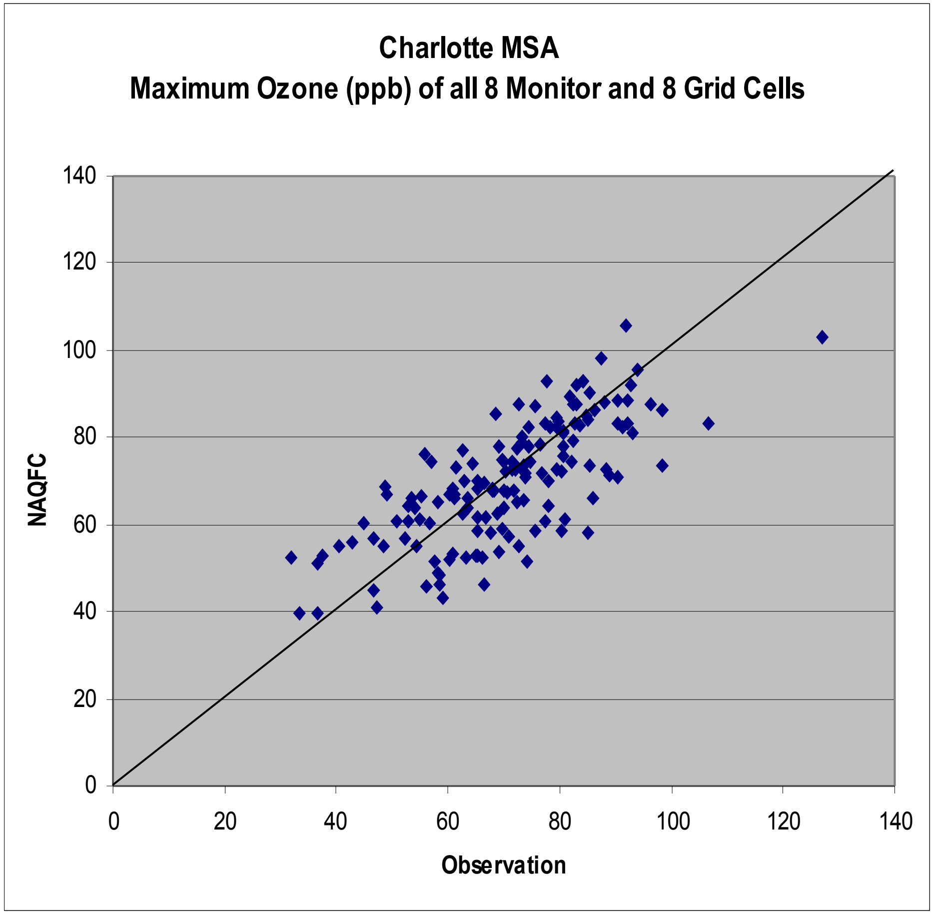


Eder et al., 2009

Modified Evaluation Approach - *Step 1*

The statistics below are based on the max. of the 8 monitors and the max. of 8 grid cells in the Charlotte MSA, where ***monitors are not matched with their grid cell.***





Period: 1 May – 30 Sept. 2007

n = 153

MB = -0.8 ppb; NMB -1.1%

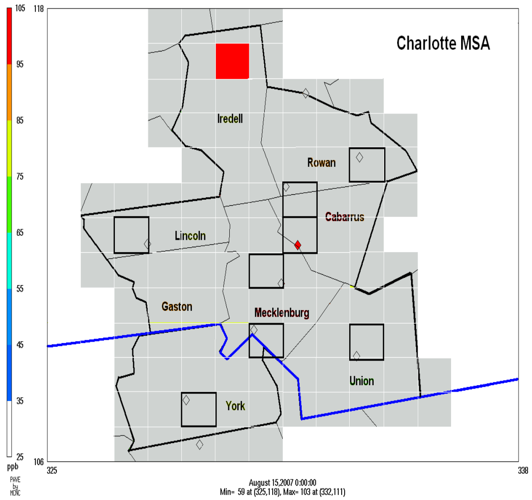
RMSE = 10.5 ppb; NME = 11.8%

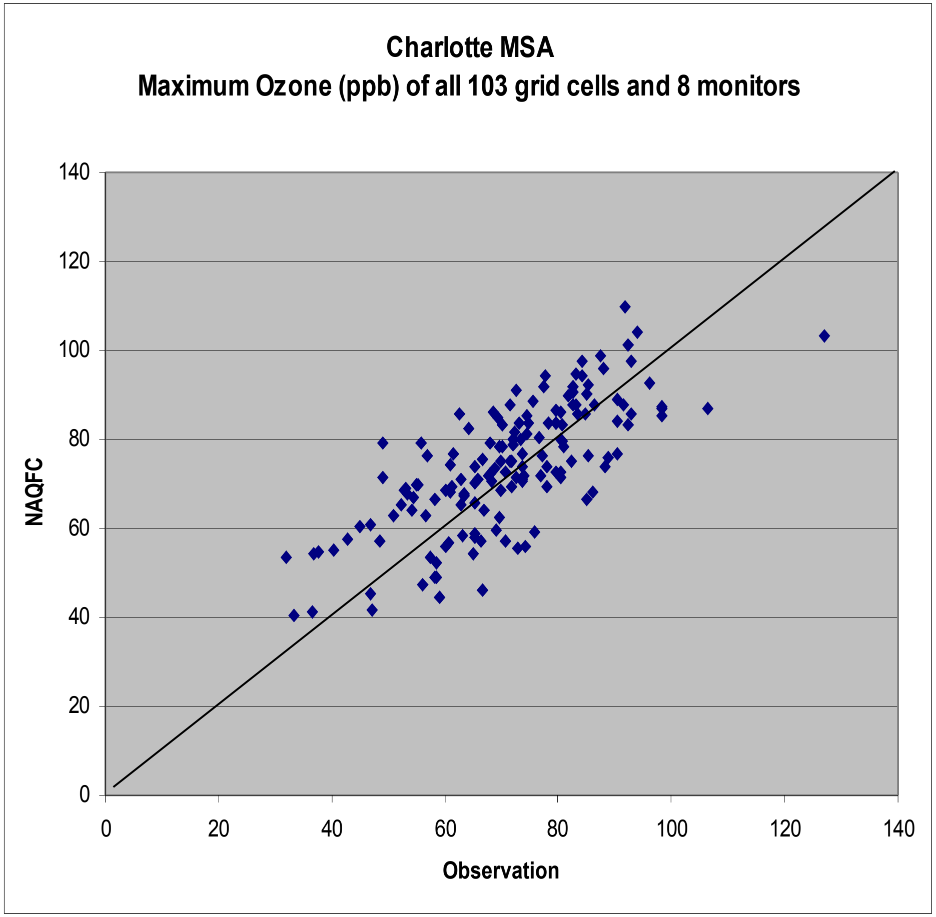
r = 0.73

Eder et al., 2009

Modified Evaluation Approach - *Step 2*

The statistics below are based on the maximum of the 8 monitors and maximum of <u>all</u> 103 model grid cells in the Charlotte MSA, where the ***monitors are <u>not</u> matched with their grid cell.***





Period: 1 May – 30 Sept. 2007

n = 153

MB = 3.1 ppb; NMB = 4.4%

RMSE = 11.0 ppb; NME = 13.1%

r = 0.74

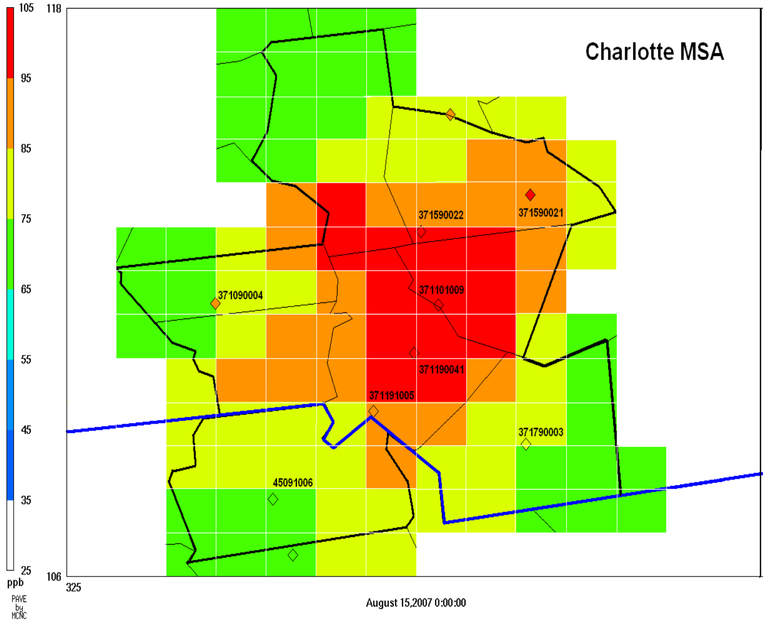
Eder et al., 2009

Evaluation Adaptation

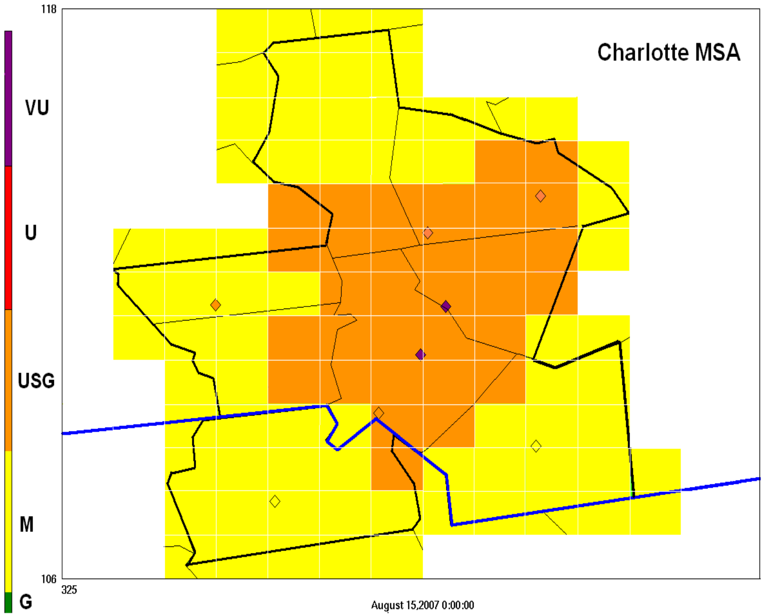
This modified, somewhat more *relaxed* evaluation approach results in “improved” statistics when compared to the more *rigid* observation vs. grid cell approach.

- We will demonstrate this approach using both:

[O_3]



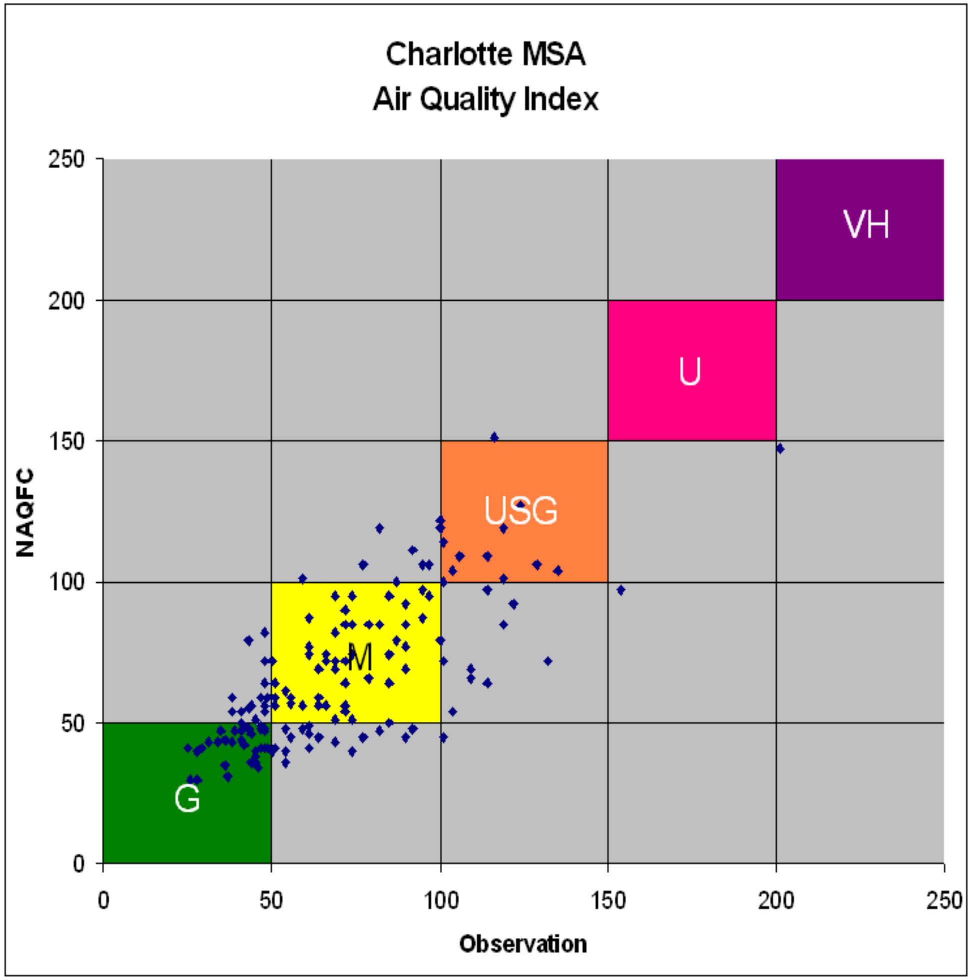
AQI



Eder et al., 2009

Modified Evaluation Approach - *Step 3*

We can take the last approach and convert the concentrations to AQI values.



Period: 1 May – 30 Sept. 2007
n = 153

MB = 6.7; NMB = 9.3%

RMSE = 22.0; NME = 25.1%

r = 0.74

Eder et al., 2009

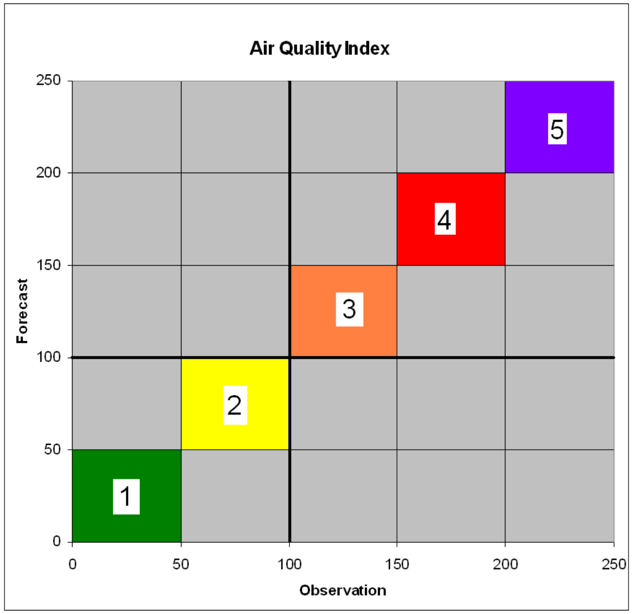
NAQFC Categorical Performance *vs.* *Human* Forecast

- Category Hit Rate: $cH_i = \dfrac{N_f^i}{N_{obs}^i}$

  where *i* is the AQI index (1, 2, 3, 4, 5) category or the color scheme (green, yellow, orange, red, purple), and

  N_f^i is the forecast instances in the *i* th category and

  N_{obs}^i is the number of observed instances in the *i* th category.



- Exceedance Hit Rate: $eH = \dfrac{N_{fo}}{N_{fo} + N_o}$

  where N_{fo} is the number of both observed and forecast exceedances (AQI ≥ 3), N_o is the number of observed, but not forecast exceedances.

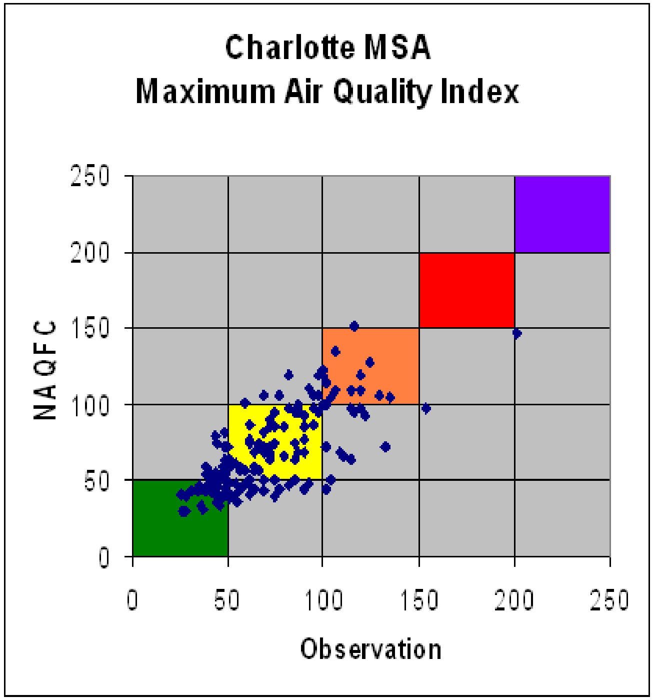
- Exceedance False Alarm Rate: $eFAR = \dfrac{N_f}{N_f + N_{fo}}$

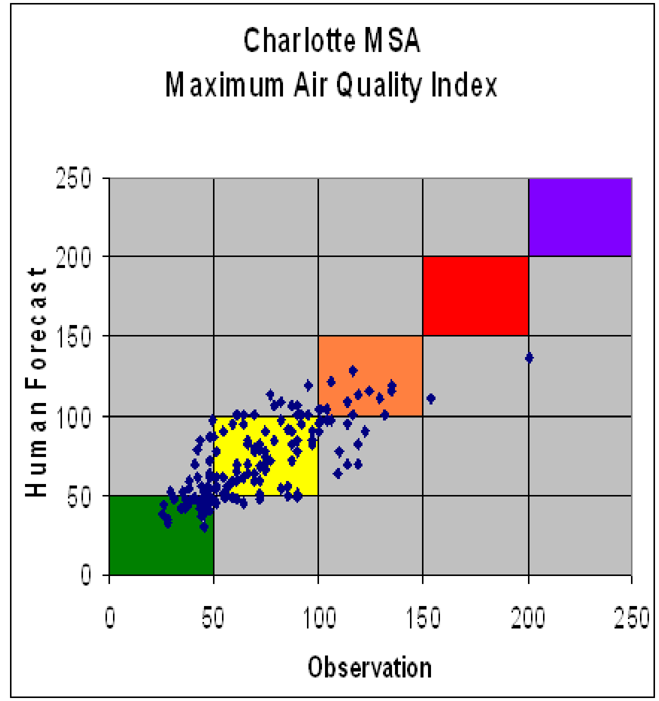
  where N_f is the number of forecast but not observed exceedances (AQI ≥ 3), N_{fo} is the number of both observed and forecast exceedances.

Eder et al., 2009

NAQFC Performance compared with *Human* Forecast*

Summer 2007





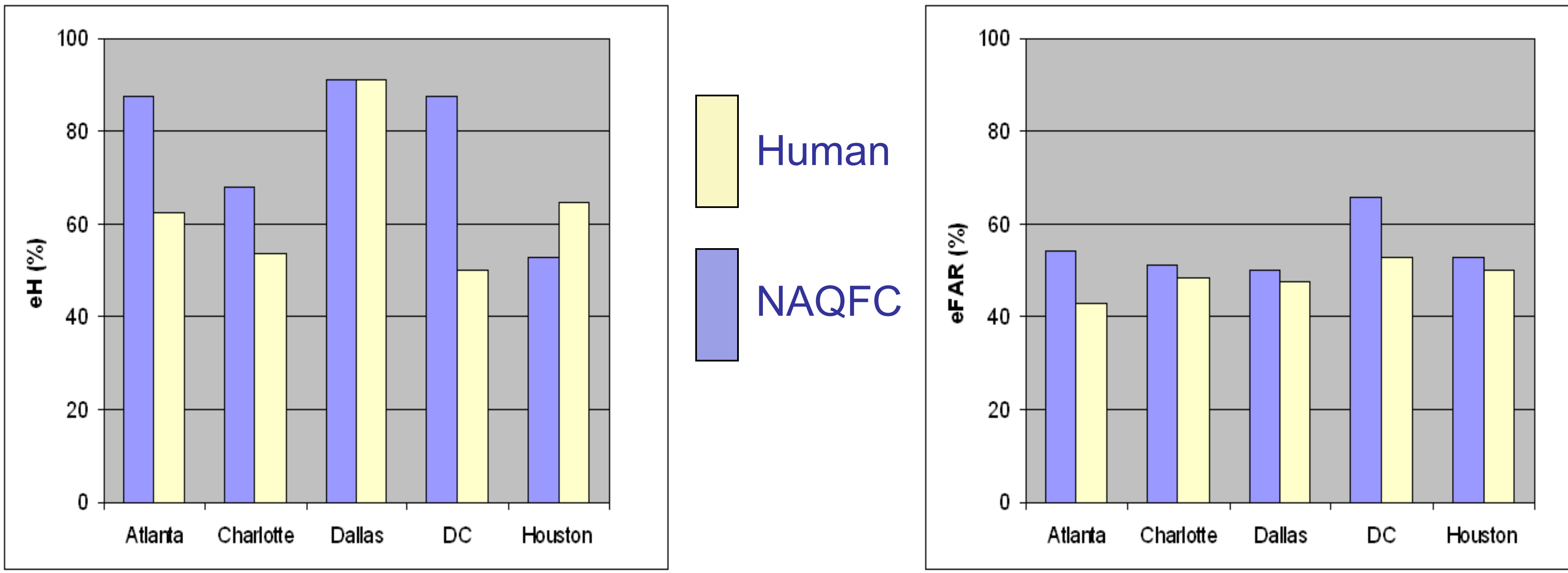
	N	r	MB	NMB	RMSE	NME
Human*	150	0.75	-0.05	-0.14	21.07	21.53
NAQFC	153	0.74	6.7	9.3	22.0	25.1

* Provided by NC Department of Environmental and Natural Resources

Eder et al., 2009

NAQFC Categorical Performance *vs. Human* Forecast

Exceedance Hit Rate **Exceedance False Alarm Rate**



Because the NAQFC is positively biased, it tends to capture a higher percentage of exceedance hit rates, but this also results in a higher percentage of false alarm rates.

Eder et al., 2009

National AQF Capability:
Next Steps

Expanding Ozone and Smoke Nationwide

- **Development of AK, HI capabilities; target operational implementation in FY10**
- **Smoke from large fires: experimental testing in AK, HI**
- **Setting the groundwork for PM: closer coupling of AQ with NAM; treatments/resolution, horizontal boundary conditions…**

Increasing Emphasis on Particulate matter components:

- **Additional components for quantitative PM forecast capability:**
  - *Objective satellite products for verification (ongoing)*
  - *Aerosols from anthropogenic source emissions in inventories: continued development/testing/analysis– testing advanced chemical mechanisms*
  - *Dust prediction*
  - *Chemical data assimilation, speciated fire emissions, closer coupling of weather and AQ simulation*

fine particles

$PM_{2.5}$

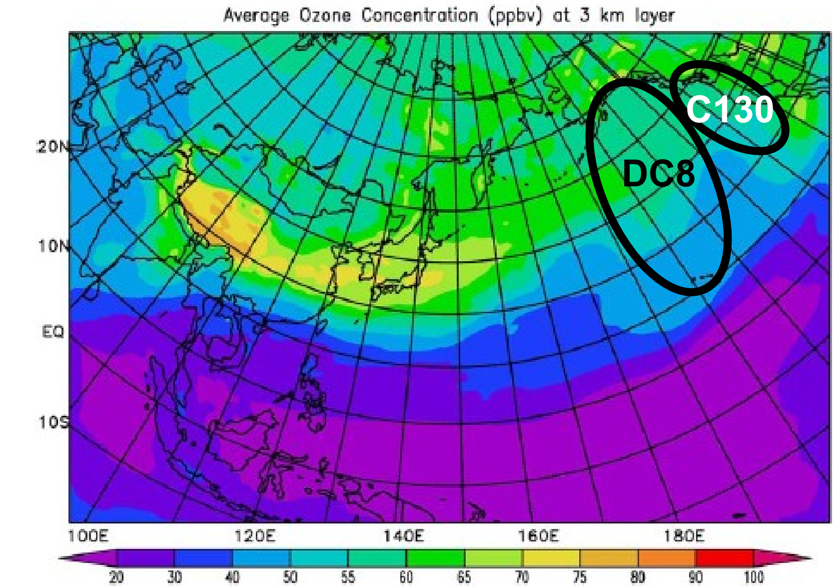
- **Integrated quantitative PM capability:**
  - *Developmental and experimental testing, to begin FY12*
  - *Target operational implementation for initial PM forecasts, NE US: FY14*
  - *Full Operational Capability, per FY09 Pres. Bud: FY15*

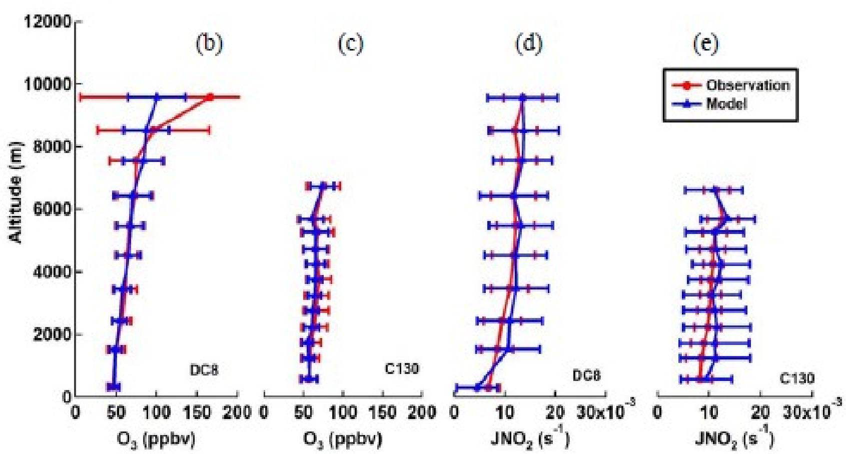
Further ahead:

- **Extend forecast range to Day 2 and beyond**
- **Include other pollutants of interest**

Slide provided by Paula Davidson

Intensive field experiments provide opportunities for comprehensive evaluations

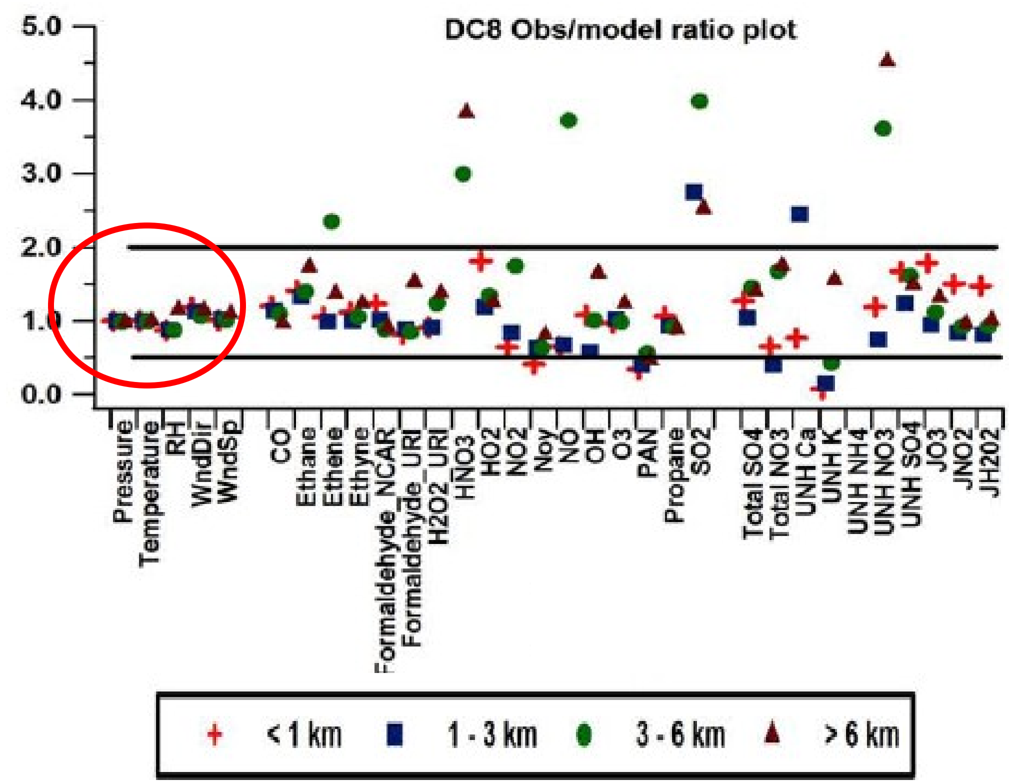




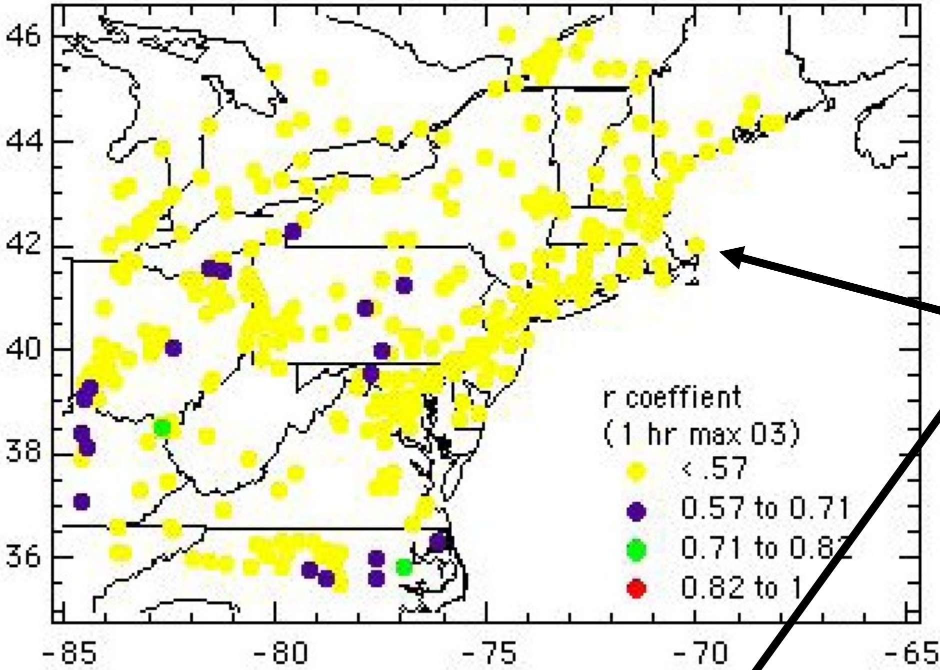
DC8 **C130**

Current CTMs Do Have Appreciable Skills In Predicting A Wide Variety Of Parameters

INTEX B – STEM Forecasts



Ensemble Forecasting of Air Quality
OZONE

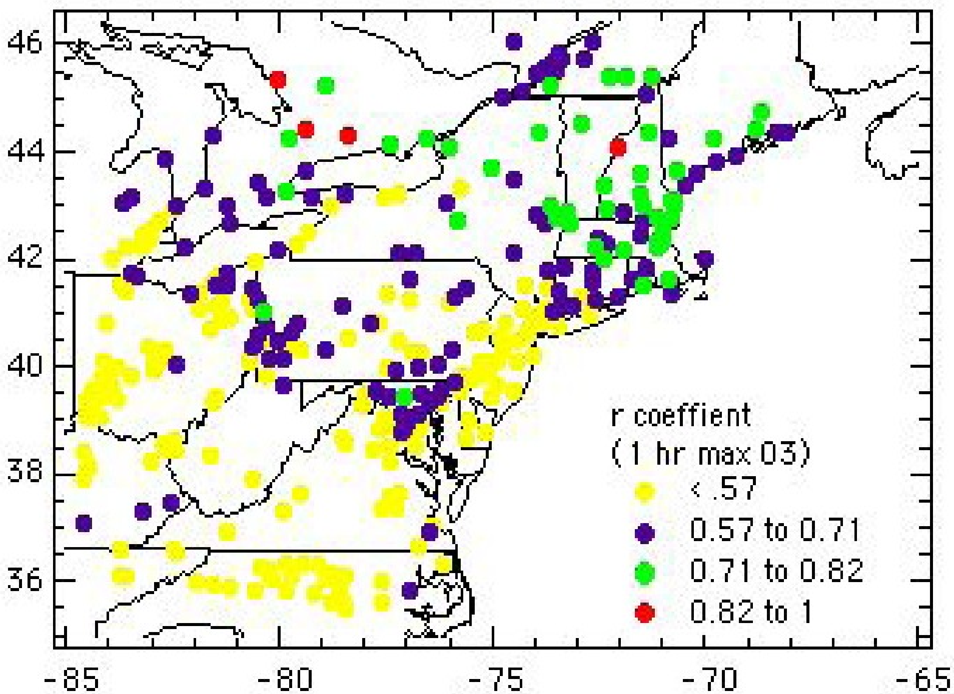


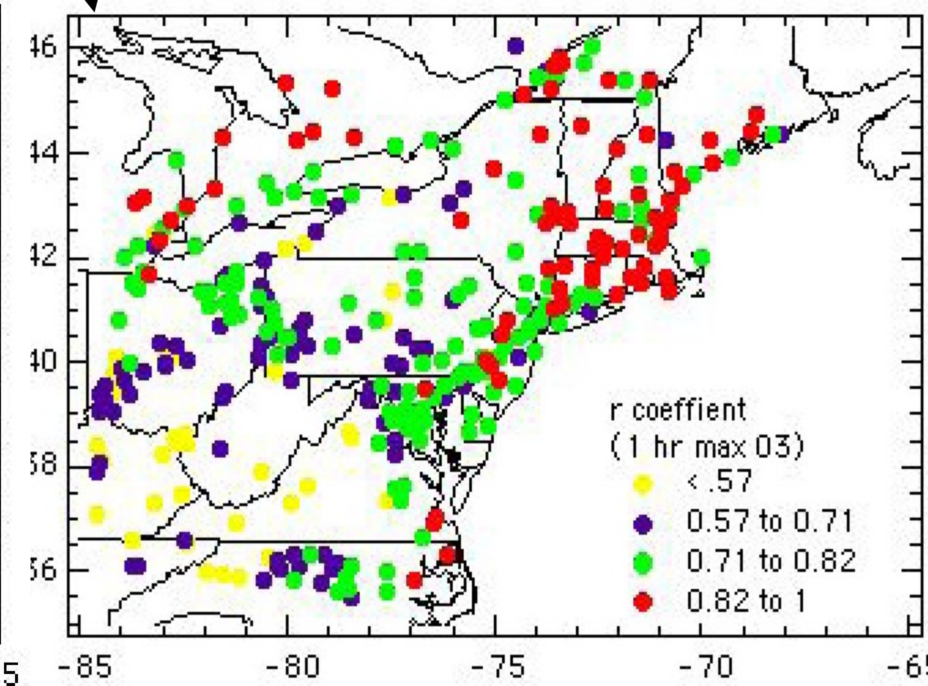
* Persistence

* Single Forward Model w/o assimilation

* Ensemble forecast (8 models) w/o assimilation (*further improvements with bias corrections based on obs*)

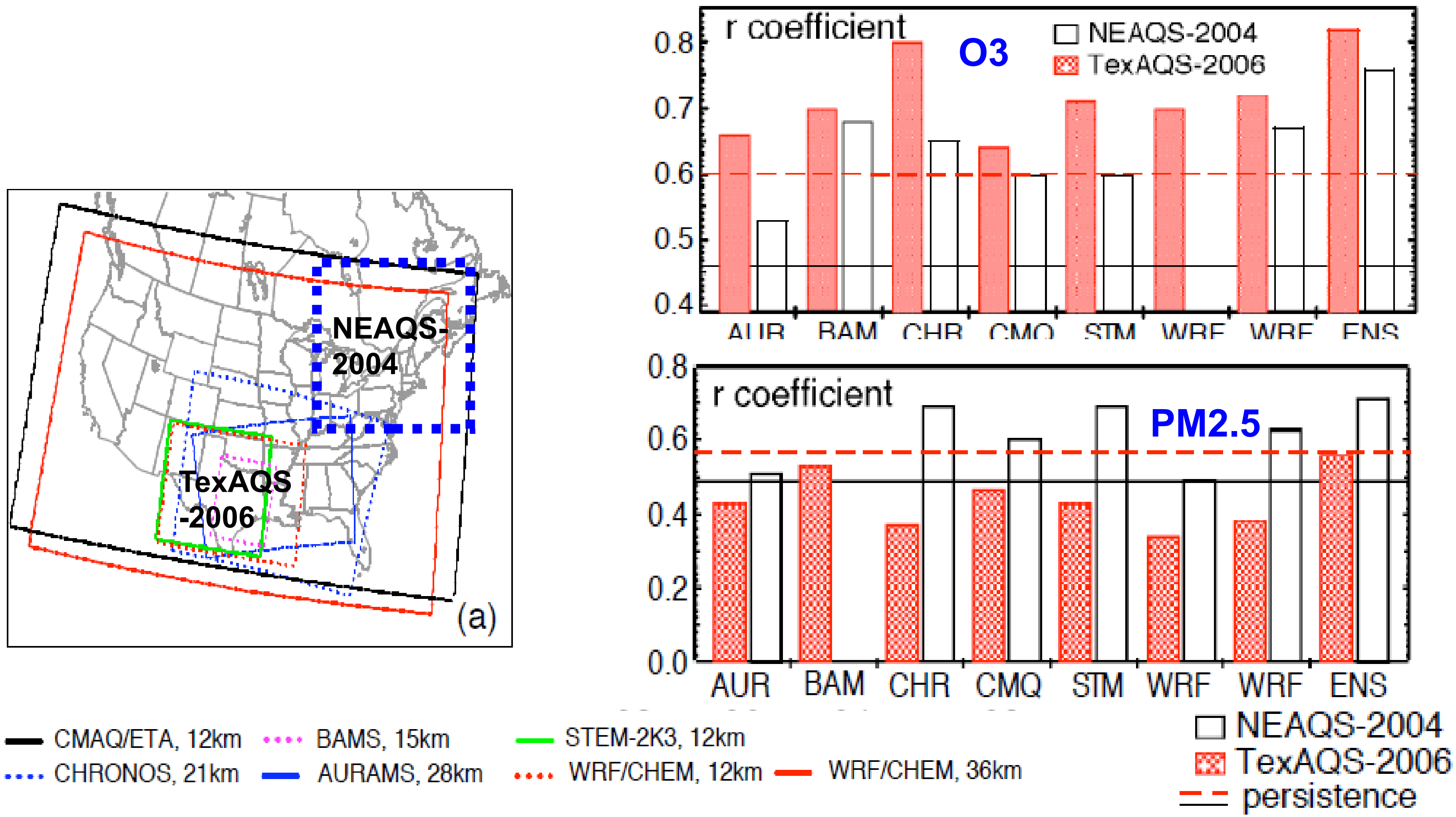
McKeen et al., JGR, 2005





Ensemble Forecast Evaluation During Major Field Experiments

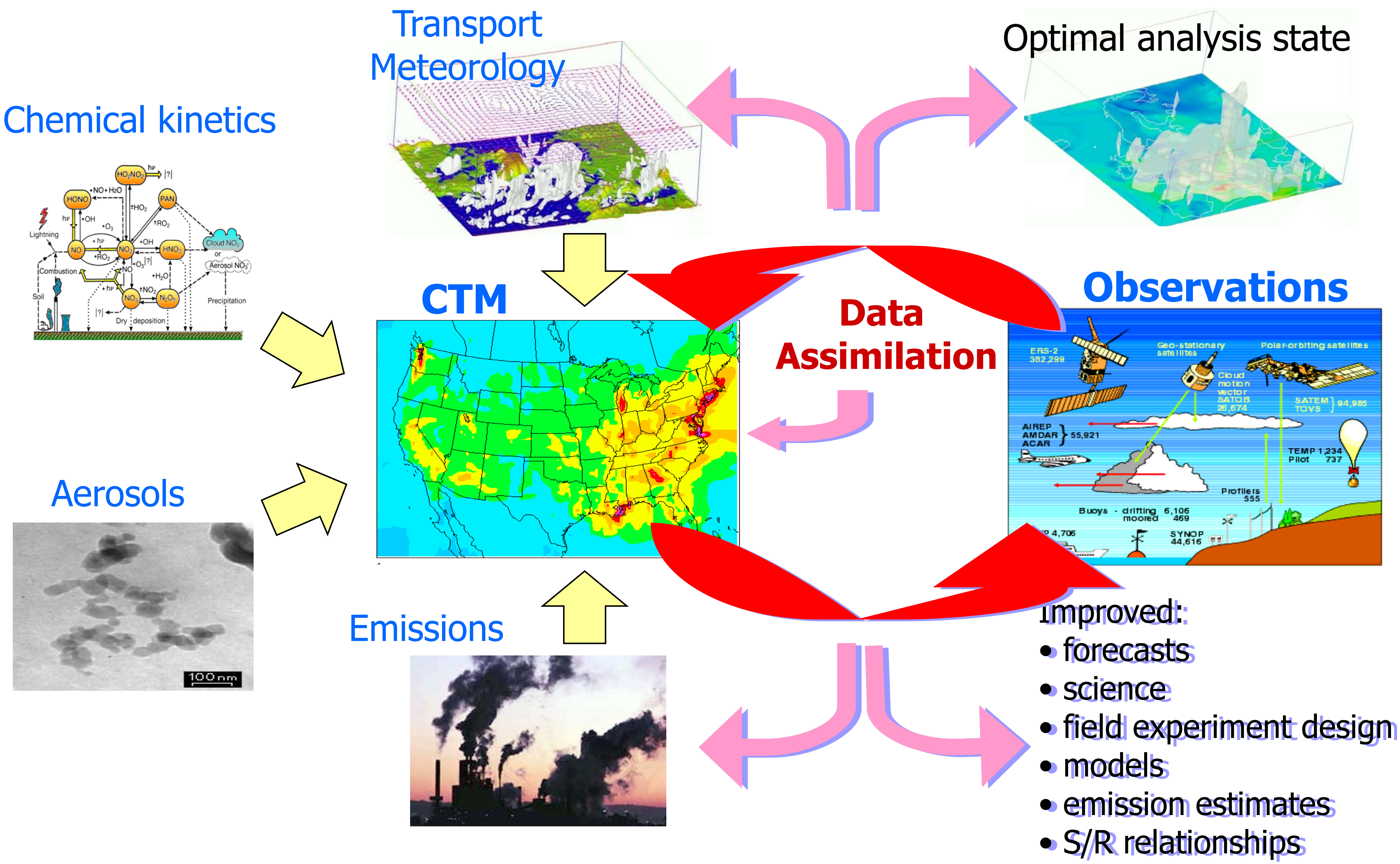
PM2.5 Remains a Challenge



McKeen et al., JGR, 2005 & 2009

Regional-Scale Chemical Analysis for Air Quality Modeling:

A Closer Integration Of Observations And Models



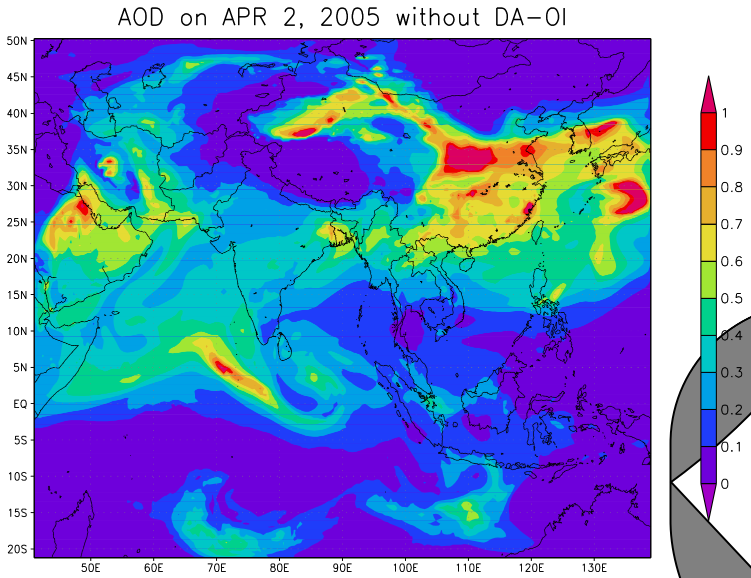
Data assimilation methods

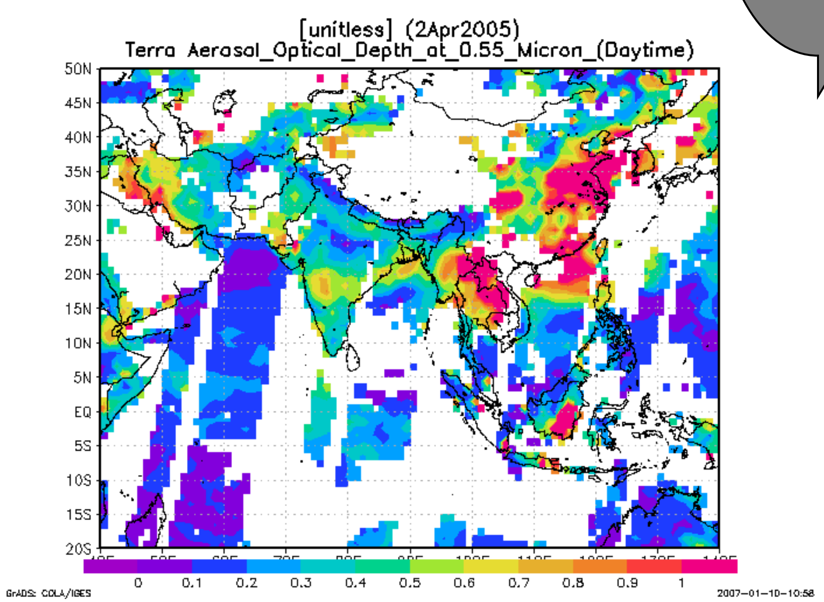
- “Simple” data assimilation methods
  - Optimal Interpolation (OI)
  - 3-Dimensional Variational data assimilation (3D-Var)
  - Kriging
- Advanced data assimilation methods
  - 4-Dimensional Variational data assimilation (4D-Var)
  - Kalman Filter (KF) - Many variations, e.g. Ensemble Kalman Filter (EnFK)

Challenges in chemical data assimilation

- A large amount of variables (~300 concentrations of various species at each grid points)
  - Memory shortage (check-pointing required)
- Various chemical reactions (>200) coupled together (lifetimes of species vary from seconds to months)
  - Stiff differential equations
- Chemical observations are very limited, compared to meteorological data
  - Information should be maximally used, with least approximation
- Highly uncertain emission inventories
  - Inventories often out-dated, and uncertainty not well-quantified

Assimilation of MODIS AOD to Produce Constrained Fields for Climate Calculations





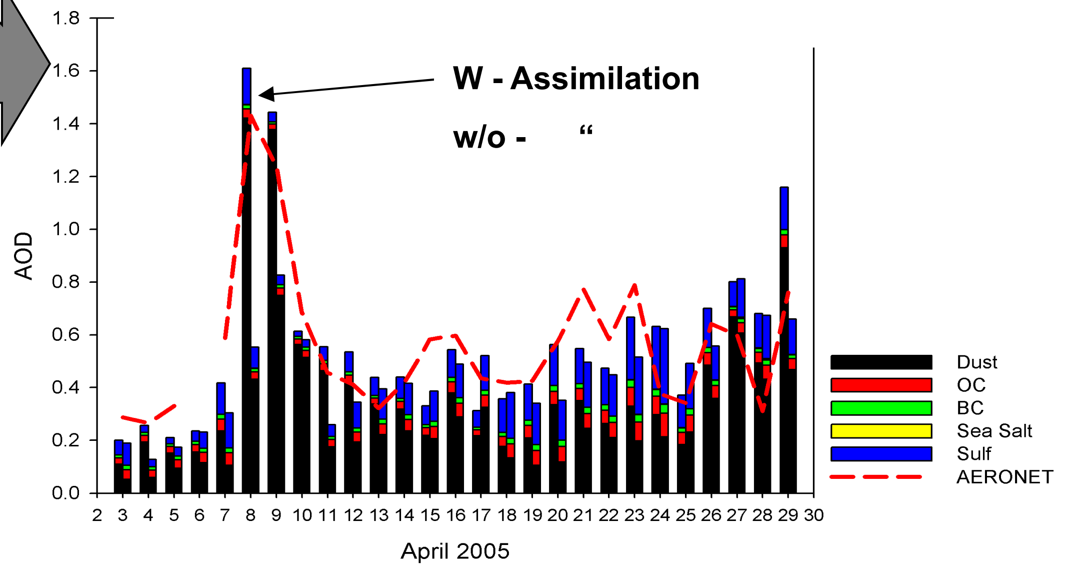
How to optimally adjust individual aerosol quantities given AOD (sulfate, BC, OC, dust, sea salt)?

- AOD by itself not unique

- Fine mode fraction helps

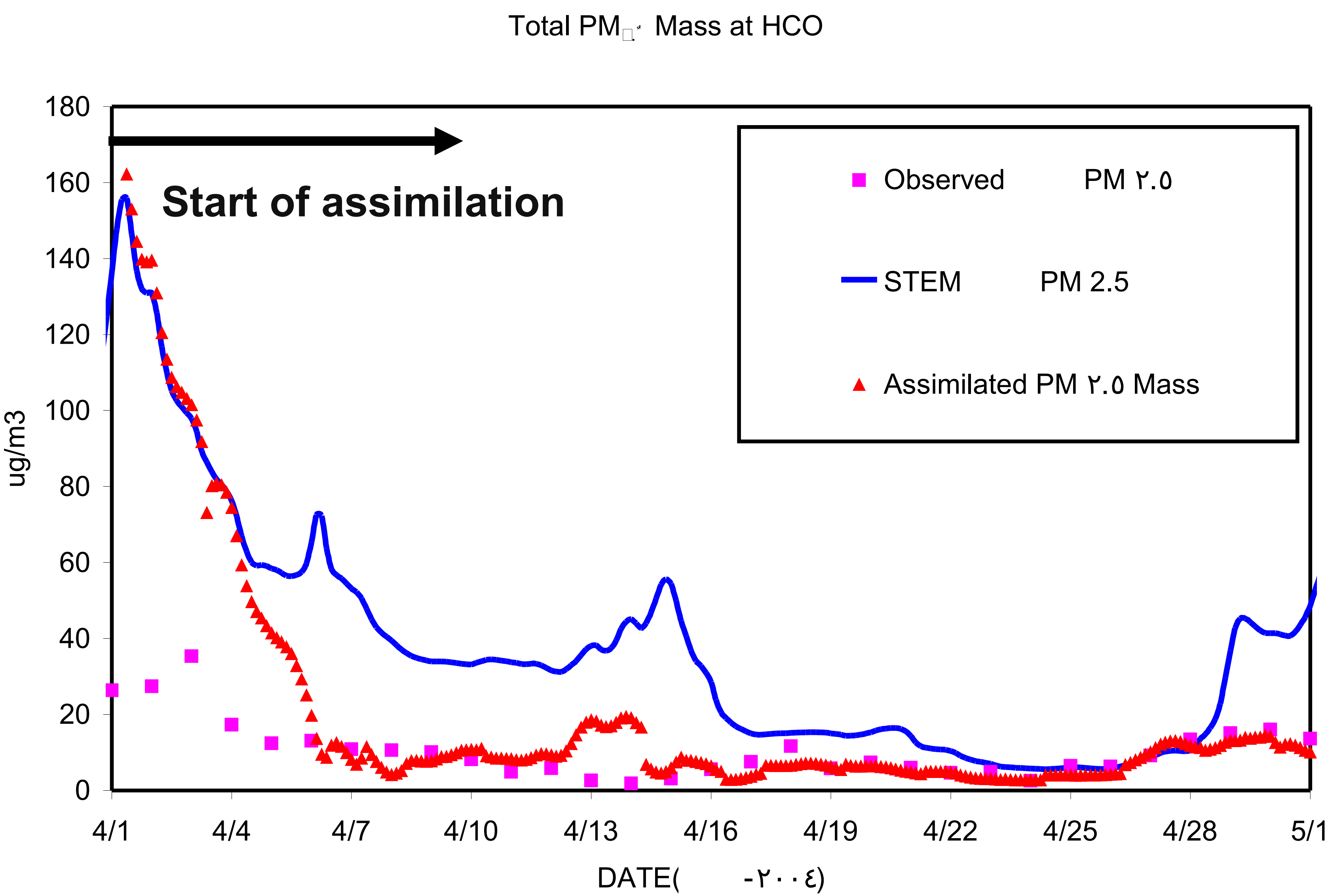
- SSA gives info to adjust abs vs scat.

Technique: Collins, W. D., et al. (2001),, *JGR*, *106*, 7313-7336



Adhikary et al., 2007,2008

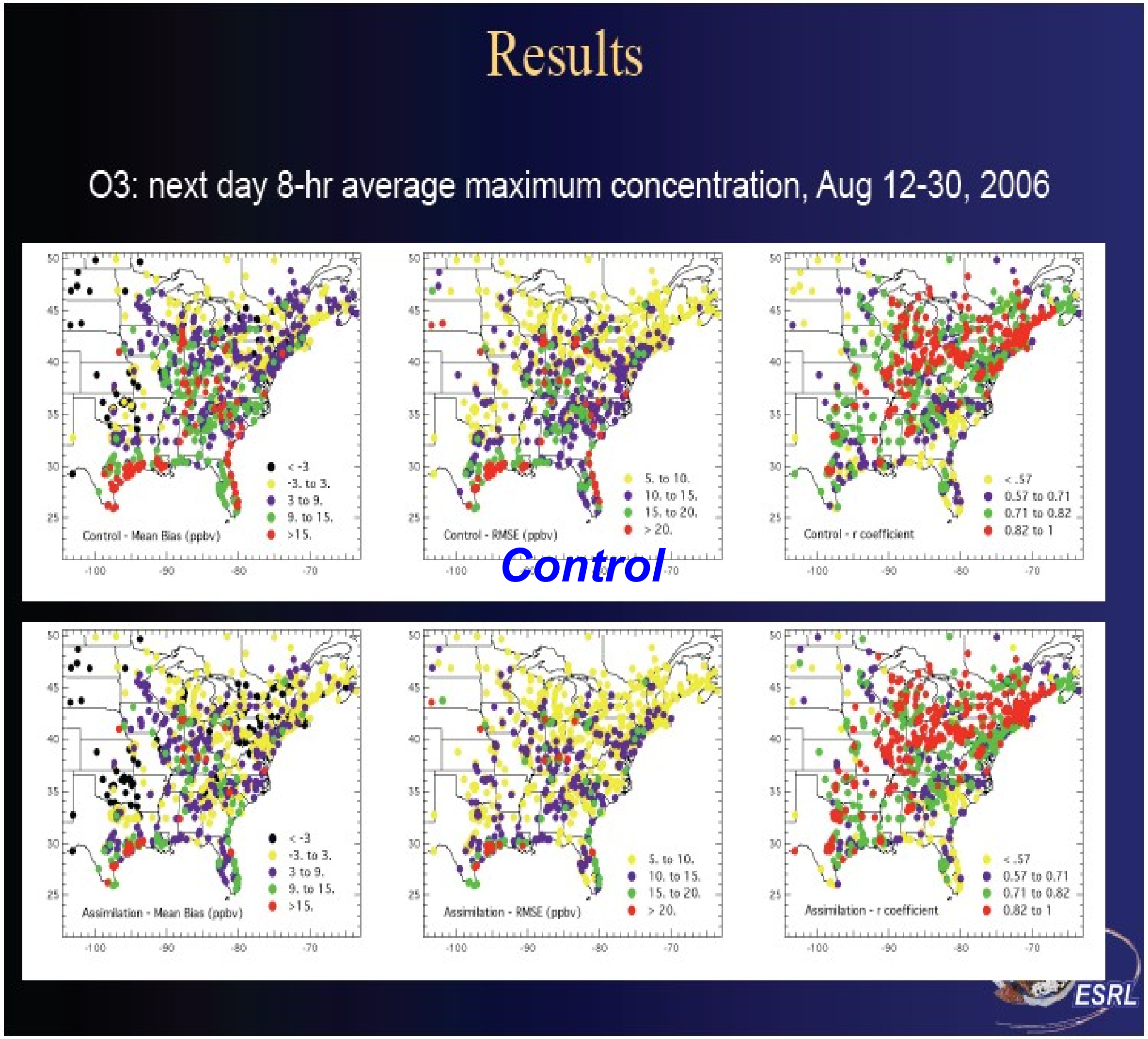
Impact of Daily MODIS Assimilation on Predicted PM 2.5 at HCO

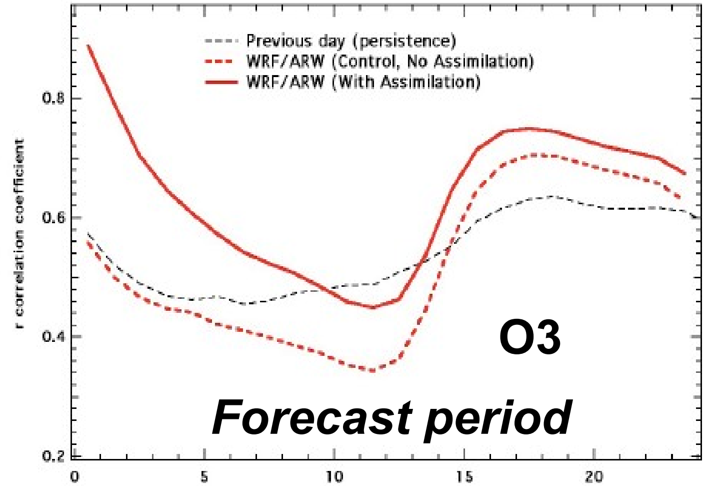


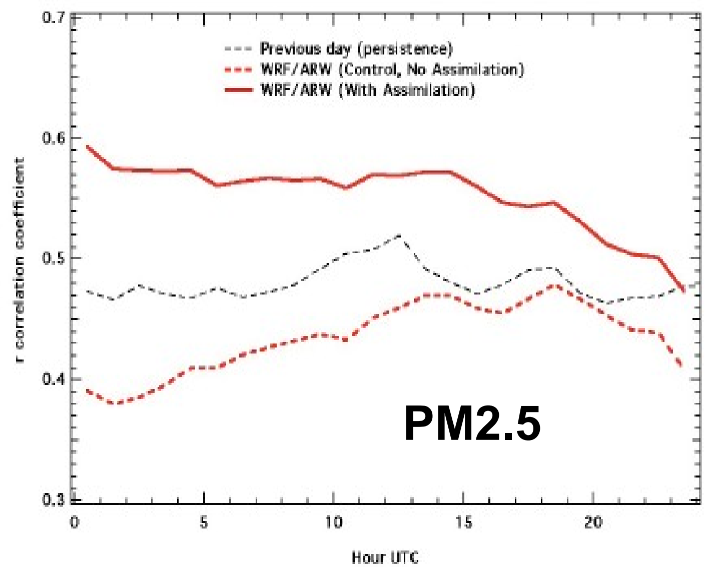
Adhikary et al., 2007,2008

ARW-WRF/Chem and the Gridpoint Statistical Interpolation (GSI) Analysis System (3dVar)

Now building a 4dvar system



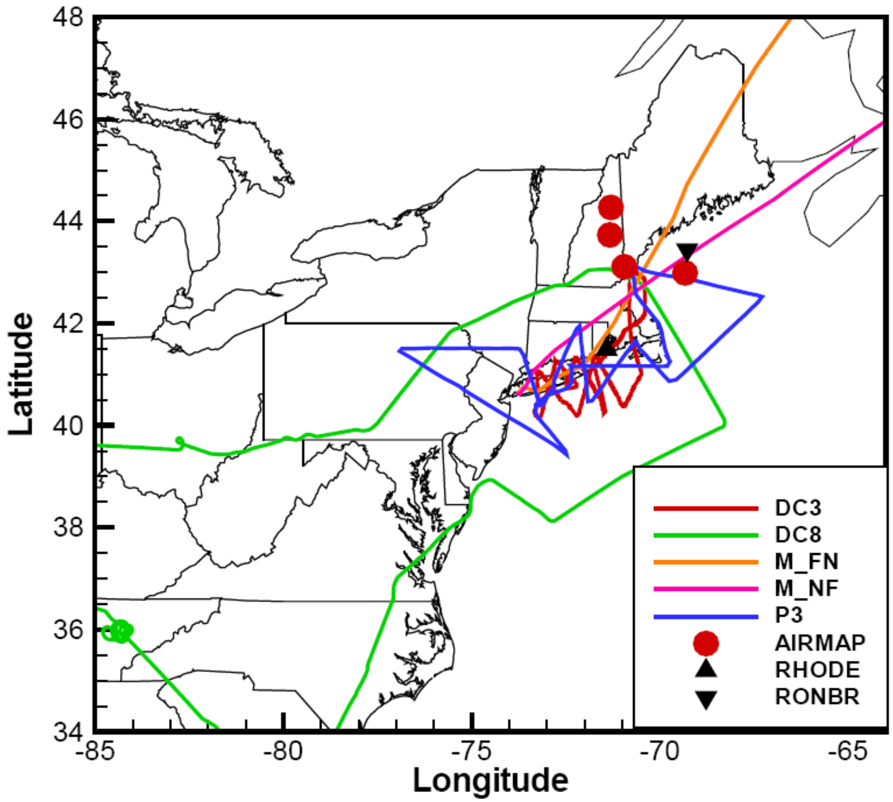




Bias **RMSE** **R**

Grell et al., 2009

Assimilation of ICARTT Ozone Observations -- Assessing Information Content



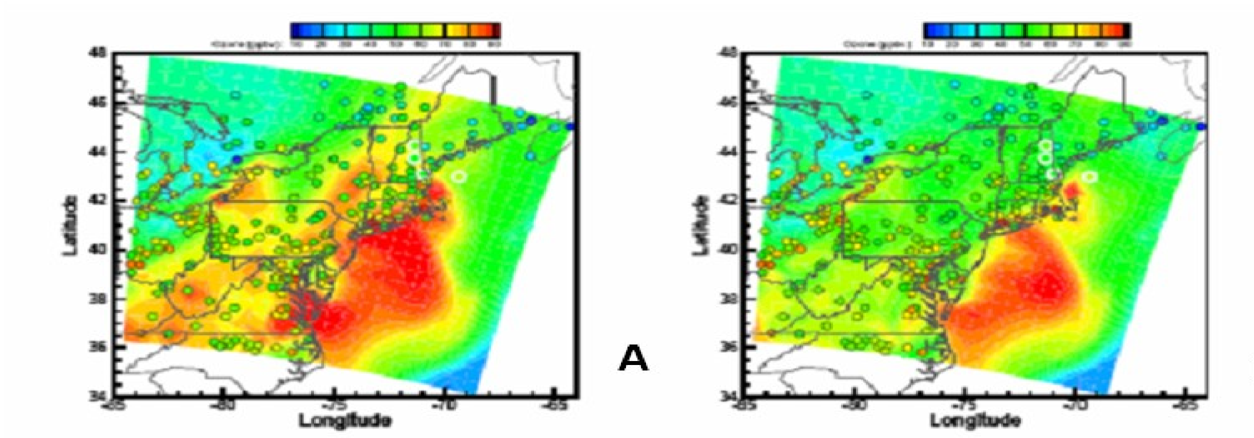
Observations	Description
AIRNOW	EPA surface stations, hourly averaged data used
DC3	Vertical profile of ozone mixing ratio from lidar
MOZ-FN	MOZAIC, Frankfurt-New York flight
MOZ-NF	MOZAIC, New York-Frankfurt flight
P3	NOAA P3-B measurement
AIRMAP	UV SPECTROSCOPY measurement at 4 sites
DC8-In	NASA In Situ Ozone via Nitric Oxide Chemiluminescence
DC8-Li	DC-8 Composite Tropospheric Ozone Cross-Sections
RHODE	Ozonesonde/Radiosonde data from Narragansett, RI
RONBR	Ozonesonde/Radiosonde data from the R/V Ronald H. Brown

Assimilation Produces An Optimal State Space

the importance of measurements above the surface!

w/o assimilation **with assimilation**

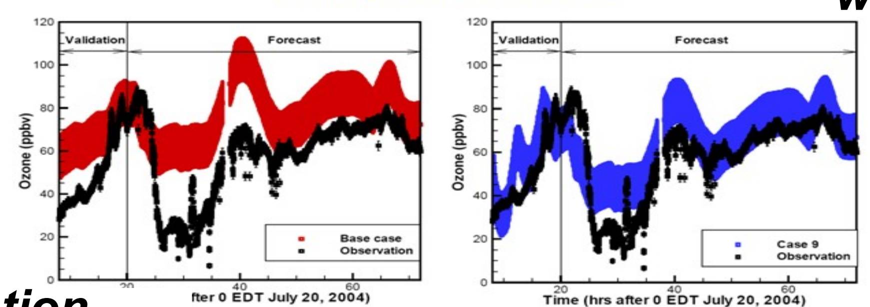
Ozone predictions



Example July 20, 2004

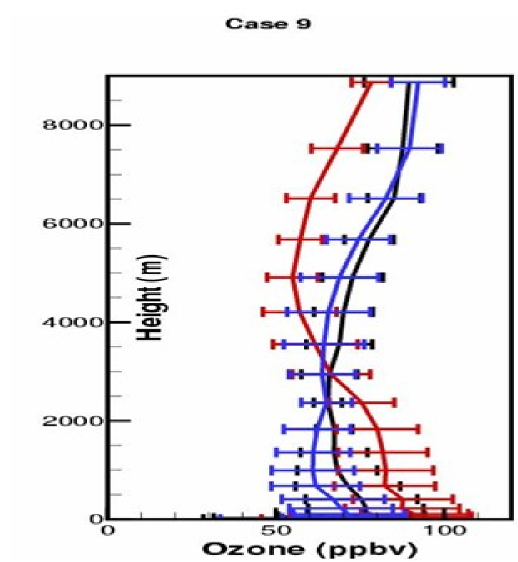
Verification: Ron Brown Observations
Independent Data

with



w/o assimilation

Predicted uncertainties estimated from background (B) error estimates



Information below 4 km most important

Region-mean profile

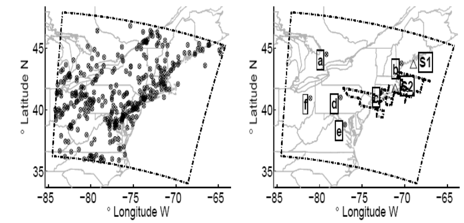
Chai et al., JGR 2007

Ensemble-based chemical data assimilation techniques can complement the variational tools

- Motivation:
  - Ensemble-based d.a. generate a statistical sample of analyses
  - Optimal state estimation applied to each member
  - Can deal effectively with nonlinear dynamics
  - Explicitly propagate (approximations of) the error statistics
  - Complement variational techniques
- Issues:
  - Initialization of the ensemble
  - Rank-deficient covariance matrix
- Contributions:
  - Models of background error covariance
  - Calculation of TESVs for reactive flows
  - Targeted observations using TESVs
  - Ensemble-based assimilation results

Challenges for reanalysis and forecasting appear to be different …. 4D-var and EnKF show promise for reanalysis

Simulation and data assimilation method	R^2 (RMS) analysis	
Best guess solution, no assimilation	0.24 (22.1)	
EnKF (50 members) "noiseless application"	0.38 (18.2)	
EnKF (200 members) "noiseless application"	0.49 (16.3)	
EnKF (50 members) adaptive multiplicative inflation	0.67 (12.7)	
EnKF (200 members) adaptive multiplicative inflation	0.82 (9.36)	
LEnKF (50 members), "noiseless application"	0.81 (9.79)	
LEnKF (50 members) adaptive multiplicative inflation	0.82 (9.52)	
LEnKF (50 members), "noiseless". Joint assimilation of state, emissions, and lateral boundary conditions	0.88 (7.75)	
LEnKF (50 members) adaptive multiplicative inflation. Joint assimilation of state, emissions, and lateral boundary conditions	0.91 (6.52)	



(a) ICARTT ground stations (b) selected stations

gure 1: Ground measuring stations (a) in support of the ICARTT campaign (340 in total), l (b) selected stations (#a–#f), two ozonesondes (S1, S2) and the flight path of a P3 plane it will be used for the numerical results/validation illustration.

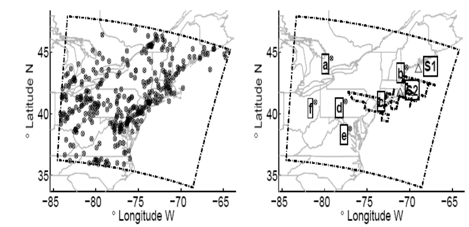
TABLE 2. Model-observations agreement (R^2 and RMS [ppbv]) for the EnKF data assimilation of only the state and of the joint state (ST), emissions (EM) and lateral boundary conditions (BC) parameters. Visible improvements in both the analysis and the forecast are obtained by adjusting the emissions and lateral boundary conditions.

Sandu et al., Quart. J. Roy. Met. Soc, 2007

Challenges for reanalysis and forecasting appear to be different …. 4D-var and EnKF show promise for reanalysis but more work is needed to impact forecasts

Simulation and data assimilation method	R^2 (RMS) analysis	R^2 (RMS) forecast
Best guess solution, no assimilation	0.24 (22.1)	0.28 (23.5)
4D-Var 50 iterations w/ AR background	0.52 (16.0)	0.29 (22.4)
EnKF (50 members) "noiseless application"	0.38 (18.2)	0.30 (23.1)
EnKF (200 members) "noiseless application"	0.49 (16.3)	0.30 (23.7)
EnKF (50 members) adaptive multiplicative inflation	0.67 (12.7)	0.19 (62.0)
EnKF (200 members) adaptive multiplicative inflation	0.82 (9.36)	0.28 (37.6)
LEnKF (50 members), "noiseless application"	0.81 (9.79)	0.34 (22.0)
LEnKF (50 members) adaptive multiplicative inflation	0.82 (9.52)	0.34 (22.0)
LEnKF (50 members), "noiseless". Joint assimilation of state, emissions, and lateral boundary conditions	0.88 (7.75)	0.42 (20.3)
LEnKF (50 members) adaptive multiplicative inflation. Joint assimilation of state, emissions, and lateral boundary conditions	0.91 (6.52)	0.40 (20.5)

TABLE 2. Model-observations agreement (R^2 and RMS [ppbv]) for the EnKF data assimilation of only the state and of the joint state (ST), emissions (EM) and lateral boundary conditions (BC) parameters. Visible improvements in both the analysis and the forecast are obtained by adjusting the emissions and lateral boundary conditions.



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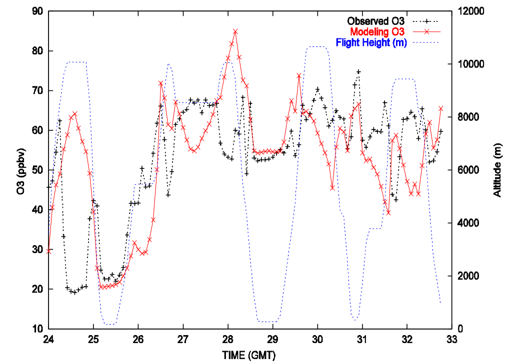
Sandu et al., QJRMS, 2007

Advanced Data Assimilation Techniques Provide Data Fusion and Optimal Analysis Frameworks

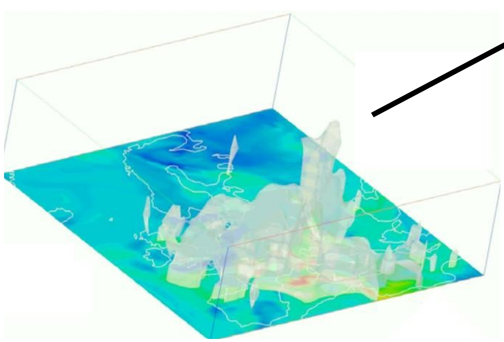
Model ~~vs.~~ + Observations

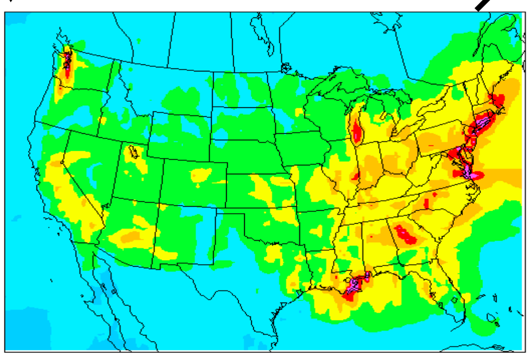


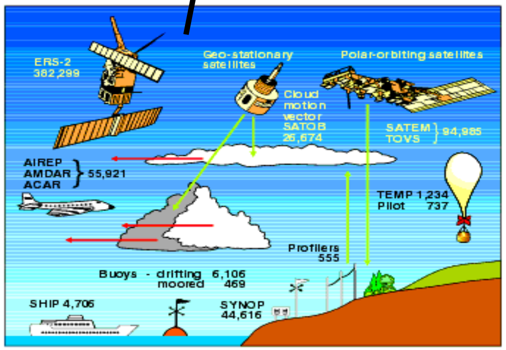
Example 4dVar:

Cost function

$$\min_{\mathbf{y}} \psi(\mathbf{y}) = \left\| \mathbf{y} - \mathbf{y}^{b} \right\|^{2}_{\mathbf{B}^{-1}} + \left\| \mathbf{H} \cdot M(\mathbf{y}) - \mathbf{o} \right\|^{2}_{\mathbf{R}^{-1}}$$







Current knowledge of the state

Model information consistent with physics/chemistry

Observations information consistent with reality

The system is very under-determined – need to combine heterogeneous data sources with limited spatial/temporal information

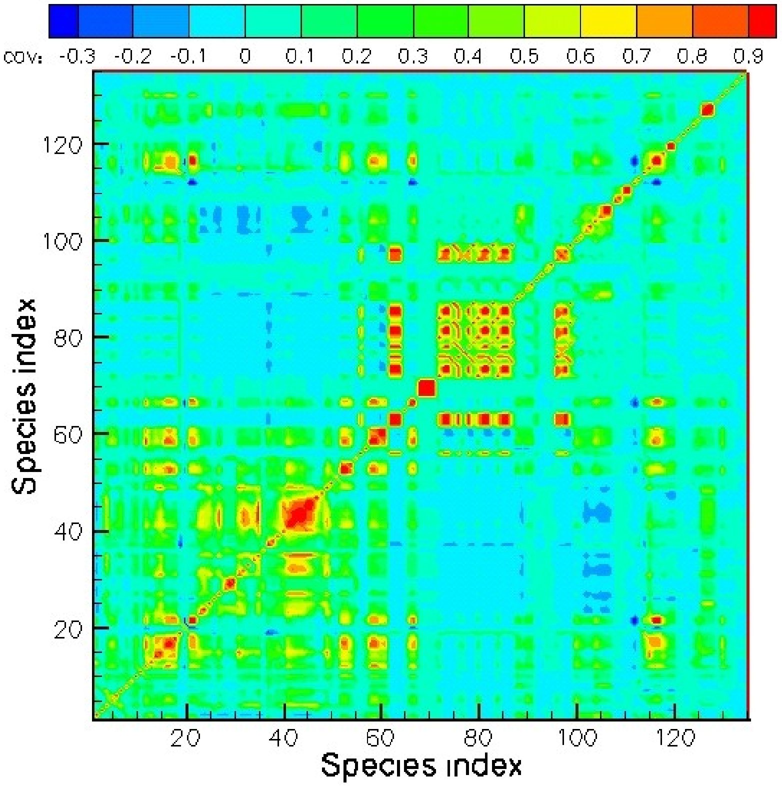
Estimation of B and O critical

NMC method (B)

$$CORR(O_3, CO) = \frac{\overline{\epsilon_{O_3} \cdot \epsilon_{CO}}}{\sqrt{\overline{\epsilon_{O_3} \cdot \epsilon_{O_3}}} \cdot \sqrt{\overline{\epsilon_{CO} \cdot \epsilon_{CO}}}}$$

- Substitute model background errors with the differences between 24hr, 48 hr, 72 hr forecasts verifying at the same time

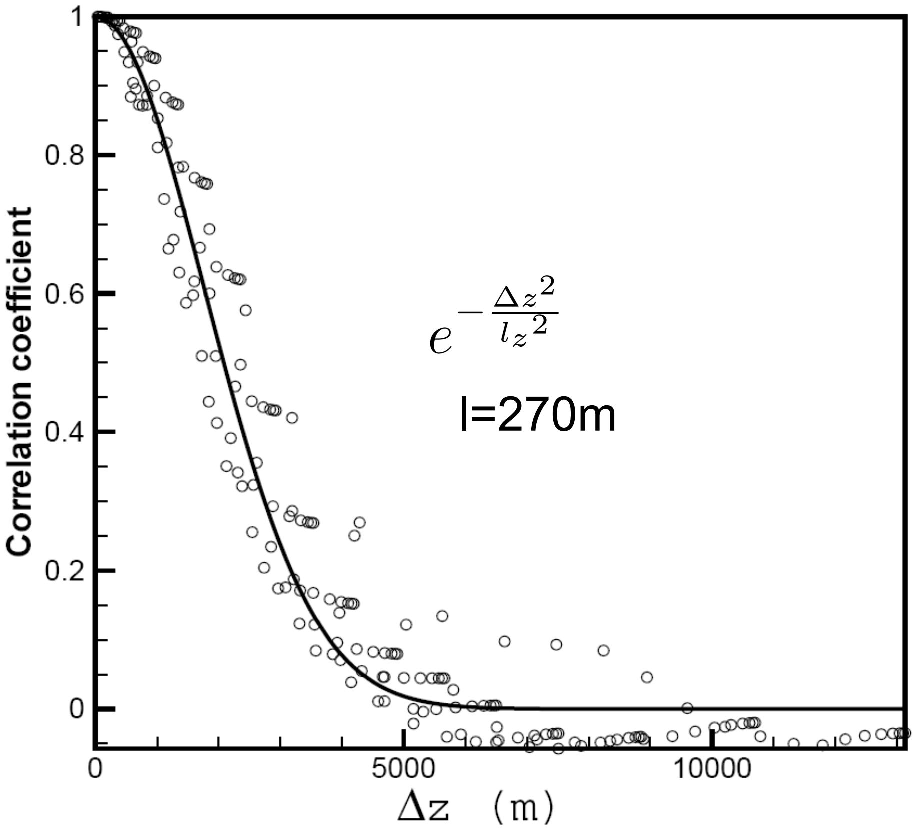
- Calculate the model background error statistics in three directions separately



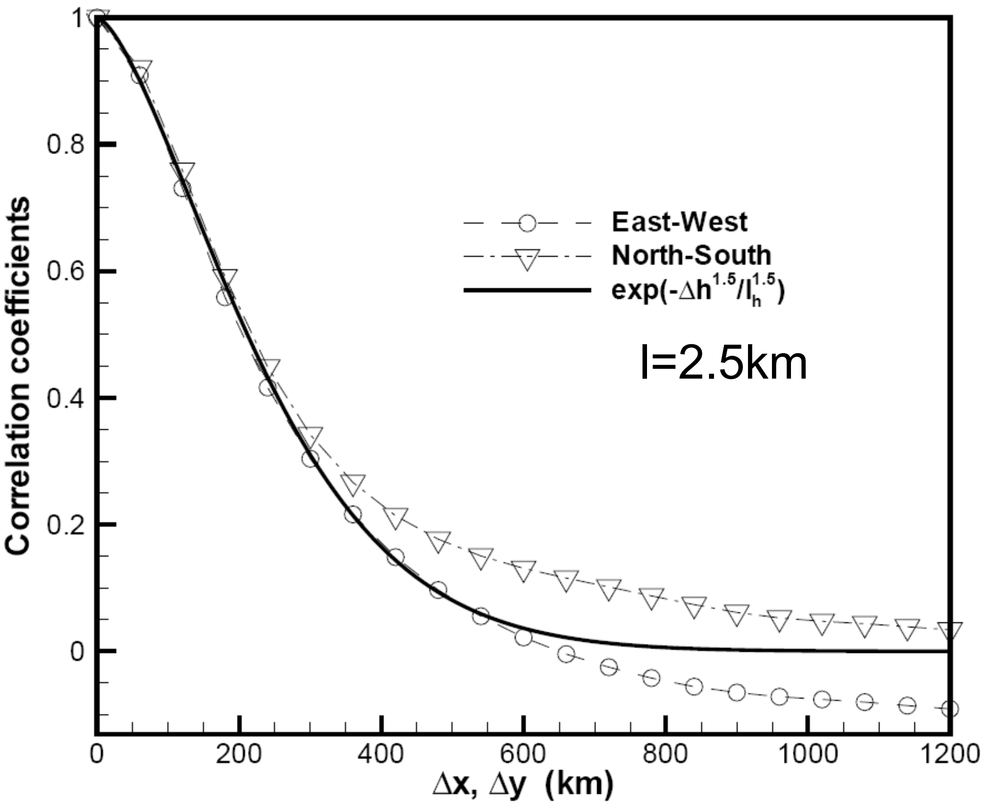
- Equivalent sample number: 811,890

NMC method results

Vertical correlation

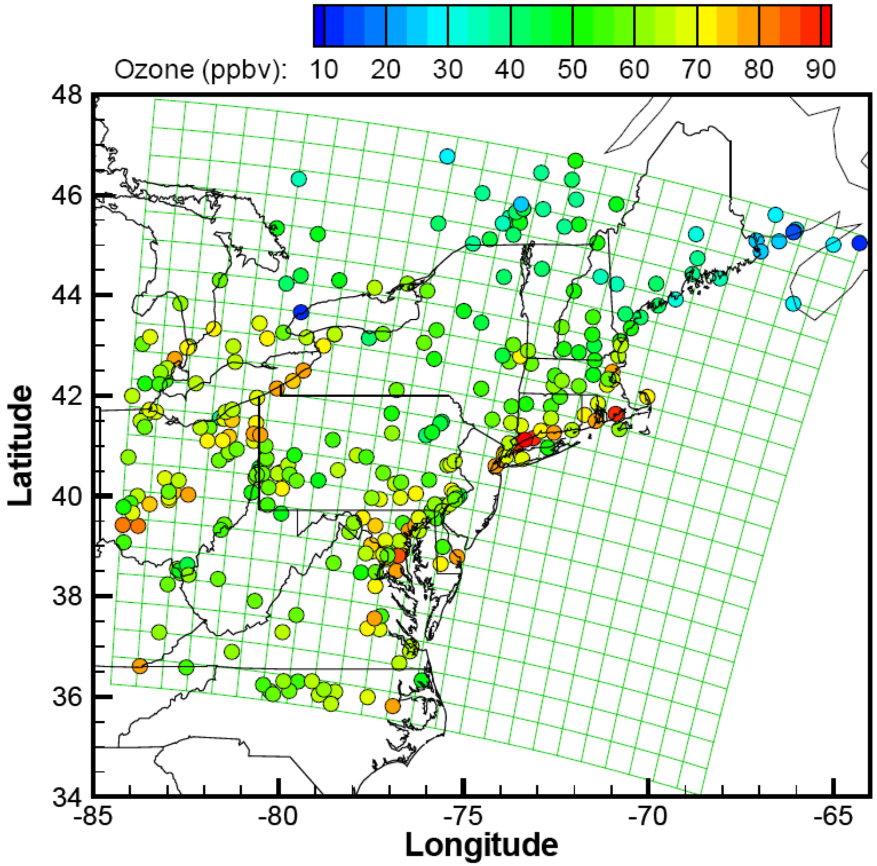


Horizontal correlation



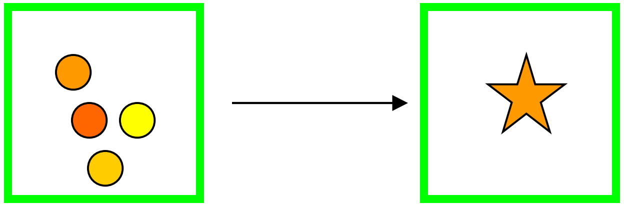
Observational error

$$J = \frac{1}{2}\left[c_0 - c_b\right]^T B^{-1}\left[c_0 - c_b\right] + \frac{1}{2}\left[y - h(c)\right]^T O^{-1}\left[y - h(c)\right]$$



Observational Error:

- Representative error
- Measurement error



Observation Inputs

- Averaging inside 4-D grid cells
- Uniform error (8 ppbv)

In AQ Predictions Emissions Are A Major Source Of Uncertainty – Data Assimilation Can Produce Optimal Estimates (Inverse Applications)

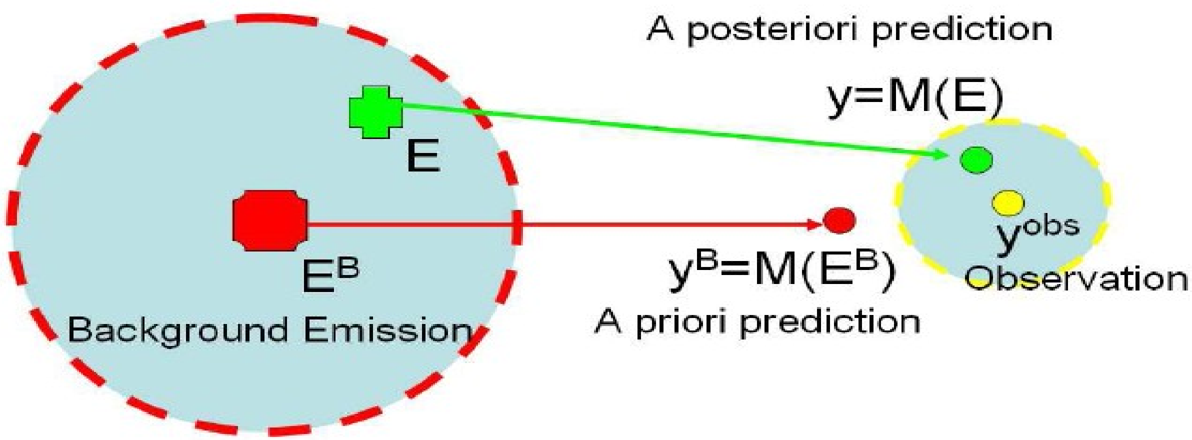


Fig. 14. A-basic methodology of top-down estimates of emissions.

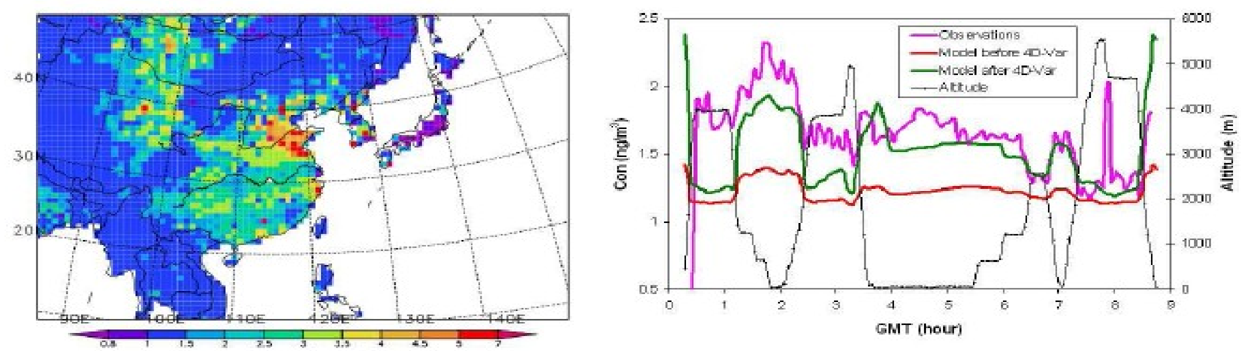
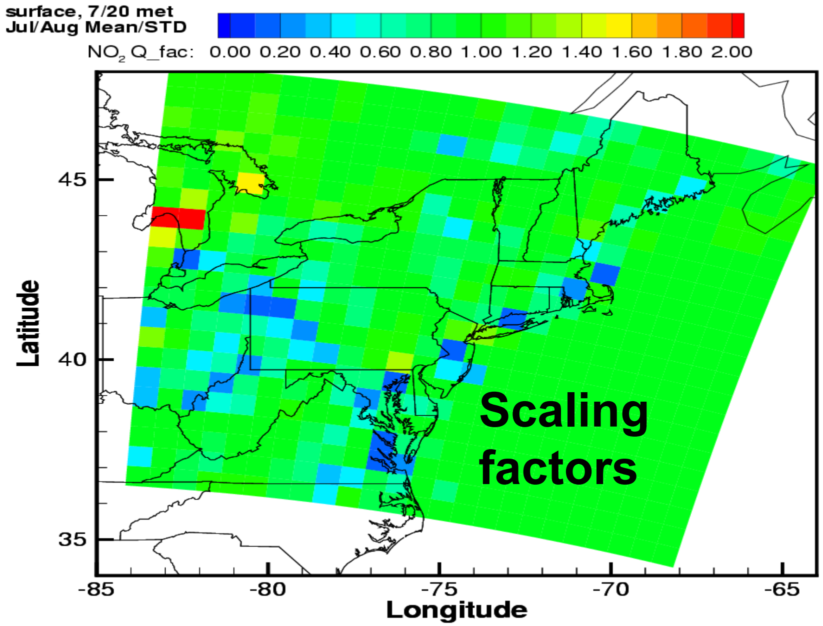


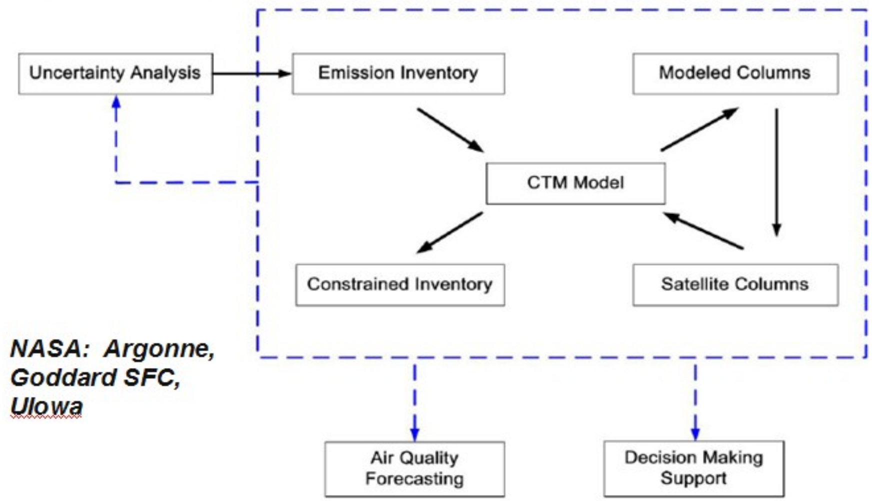
Fig. 15. Optimal mercury emission scaling factors obtained using the 4D-Var approach and the mercury measurements on board the C-130 during the Ace-Asia experiment. Results are for a month-long assimilation window (April 2001).

Li et al., Atmos. Env., 2007

Rapid Updates of Emissions Are Needed



We are developing new approaches to integrate satellite data with chemical transport models and emission inventories for improved AQM



4D-Var setup:

Time window:

July , 2004

Control:

Initial ozone, and NOx emissions

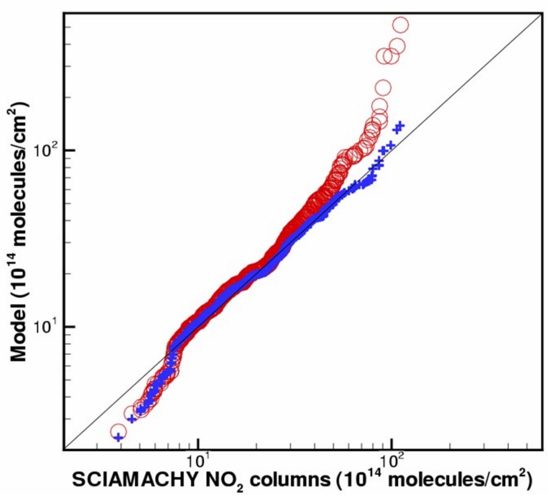
Observations:

Ozone from different platforms, and SCIAMACHY tropospheric NO_2 columns

Emission changes over domain (ratio of new emission over NEI01)

Case	Surface (level 1)	Elevated (2 & above)	Total (all levels)
1 E only	0.934	0.849	0.920
2 E & IC	0.928	0.881	0.908
"OI"	1.318	1.030	1.246

Quantile-quantile plot



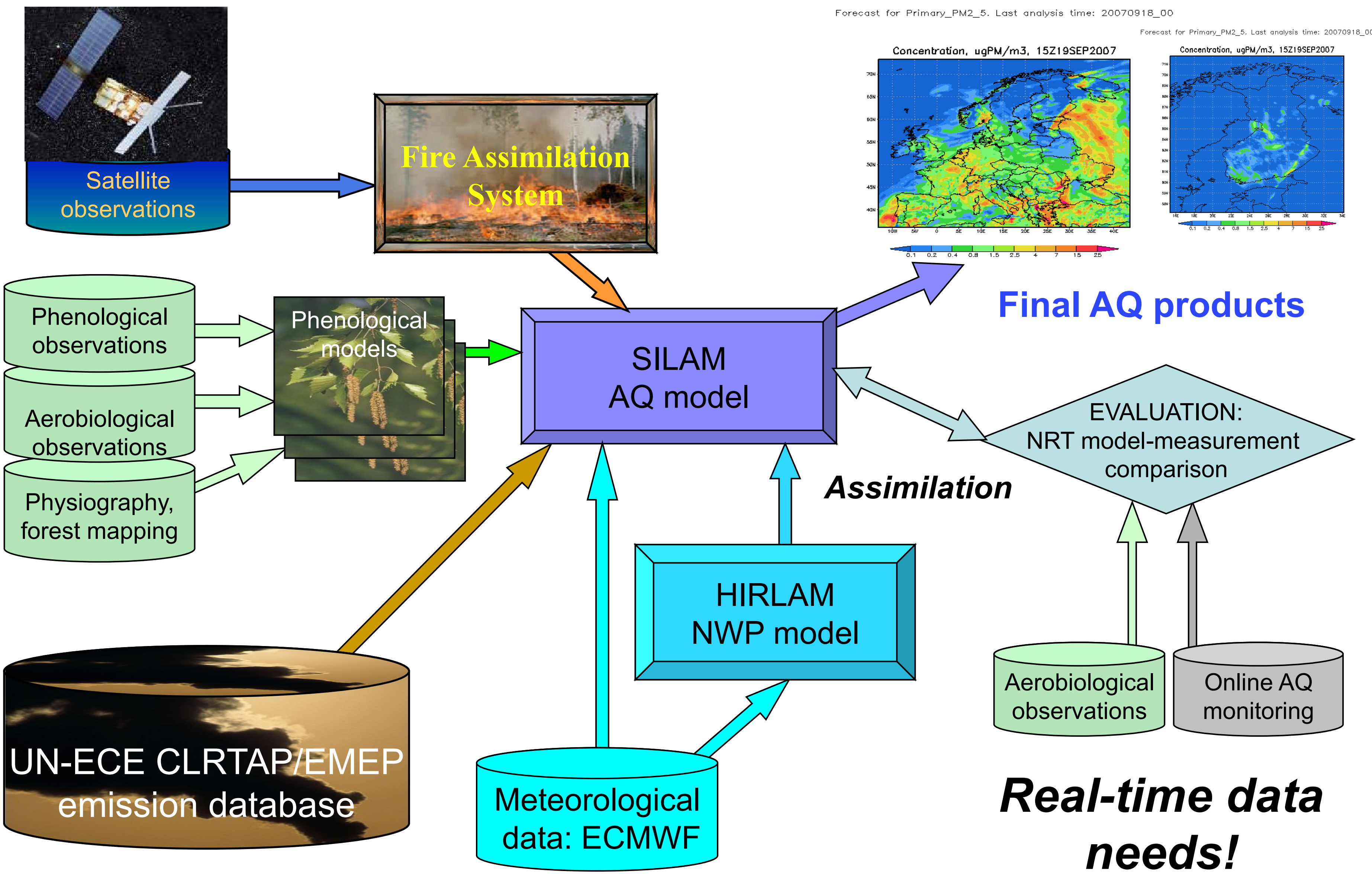
Blue:

After NOx Emission adjustmentent

Red:

Before NOx Emission adjustmenter

Many Meteorological Services Already Supply Operational Chemical Weather Products (e.g., FMI)



Phased Testing for Transition to Operations

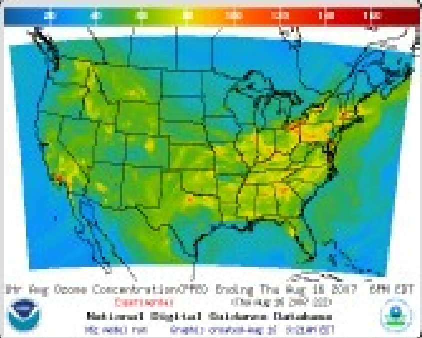
Phased Testing

Research
Does the science work?

Developmental Testing
Does it work with operational systems?

Experimental Testing
Does it meet deployment readiness criteria?

Deploy into Operations



Key S&T Tests
O_3 -- Summer 2007

More advanced PBL mixing in CMAQ (CB05)

PBL mixing (ACM2) in CMAQ, CA off-road emissions, dry deposition upgrades

NAM and emissions data updates; Plume rise correction

Section 13
Developing a Forecasting Program

Understanding Users' Needs

Understanding the Processes that Control Air Quality

Choosing Forecasting Tools

Data Types, Sources, and Issues

Forecasting Protocol