

# Regional Chemical Modeling in Support of ICARTT

## Topics:

- How good were the regional forecasts?
- What are we learning about the emissions?
- What are our plans for integrating models with observations?

# Our Analysis Framework

**MOZART Global Chemical Transport Model**

**Mesoscale Meteorological Model (RAMS or MM5)**

**Influence Functions  
Emission Biases/  
Inversion**

**Meteorological Dependent Emissions (biogenic, dust, sea salt)**

**Anthropogenic & biomass burning Emissions**

**TOMS O<sub>3</sub>**

**STEM Tracer Model (classified tracers for regional and emission types)**

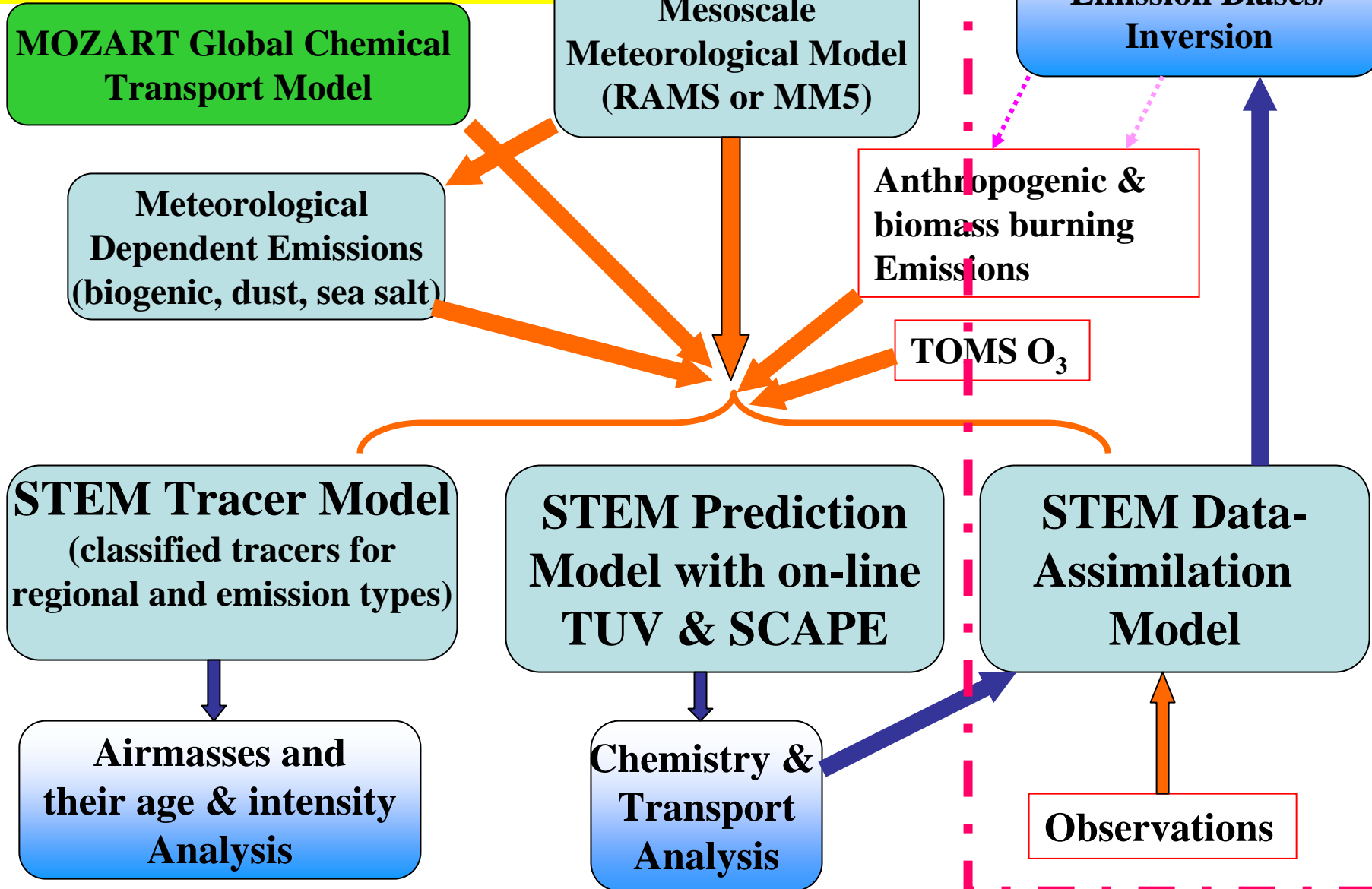
**STEM Prediction Model with on-line TUV & SCAPE**

**STEM Data-Assimilation Model**

**Airmasses and their age & intensity Analysis**

**Chemistry & Transport Analysis**

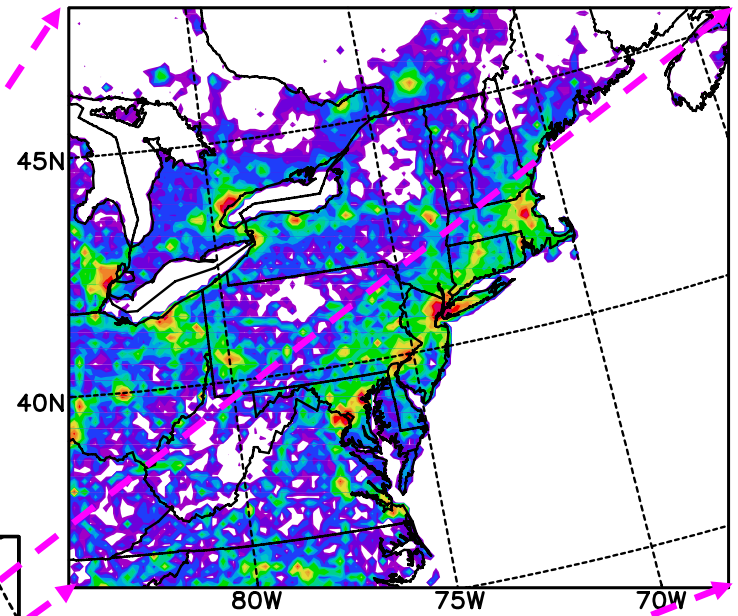
**Observations**



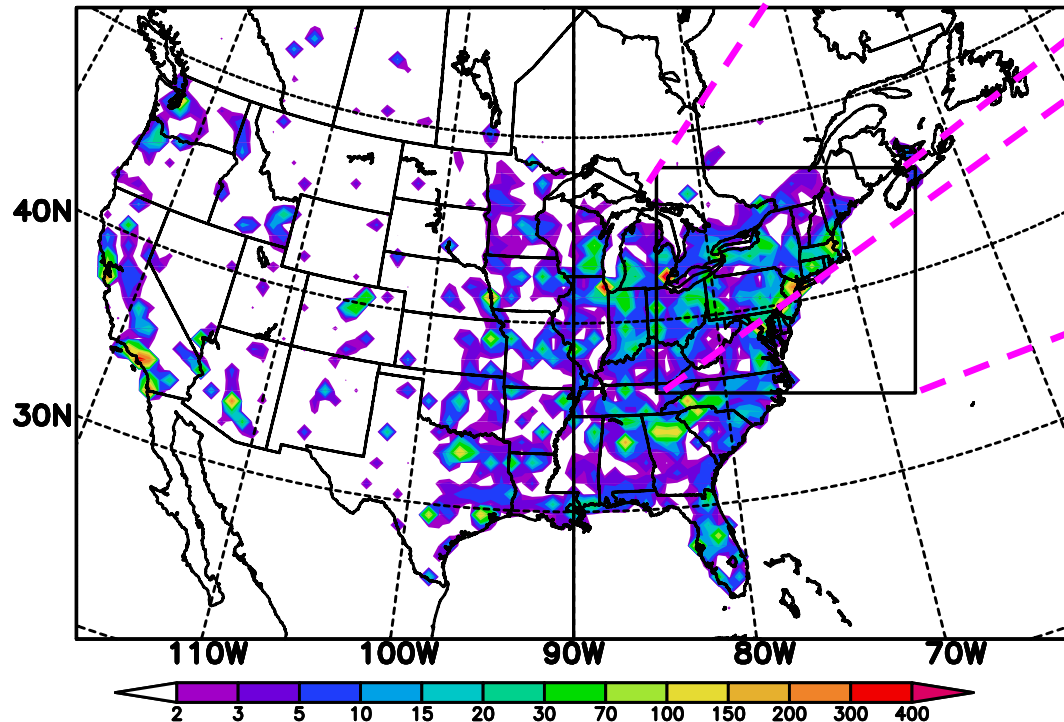
# Analysis Done at 60 and 12 km Horizontal Resolution

NEI-1999 emission in 60km (below)  
and 12km (right) domains.

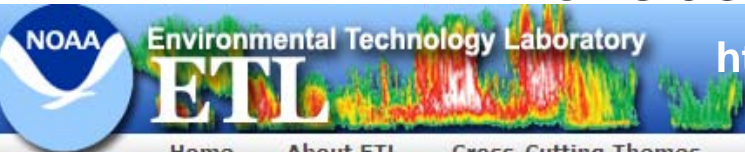
Mean CO Emission for Typical Summer day ( $10^{11}$  Molecules/cm<sup>2</sup>/s)



Mean CO Emission for Typical Summer day ( $10^{11}$  Molecules/cm<sup>2</sup>/s)



# Extensive Real-Time Evaluation of Regional Forecasts – *Stu McKeen*



<http://www.etl.noaa.gov/programs/2004/neaqs/verification/>

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Select the model cycle initialization:

00Z Jul 13  
12Z Jul 13

**Sites**

Select site type:

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- Chemistry
- Mobile

Select site location:

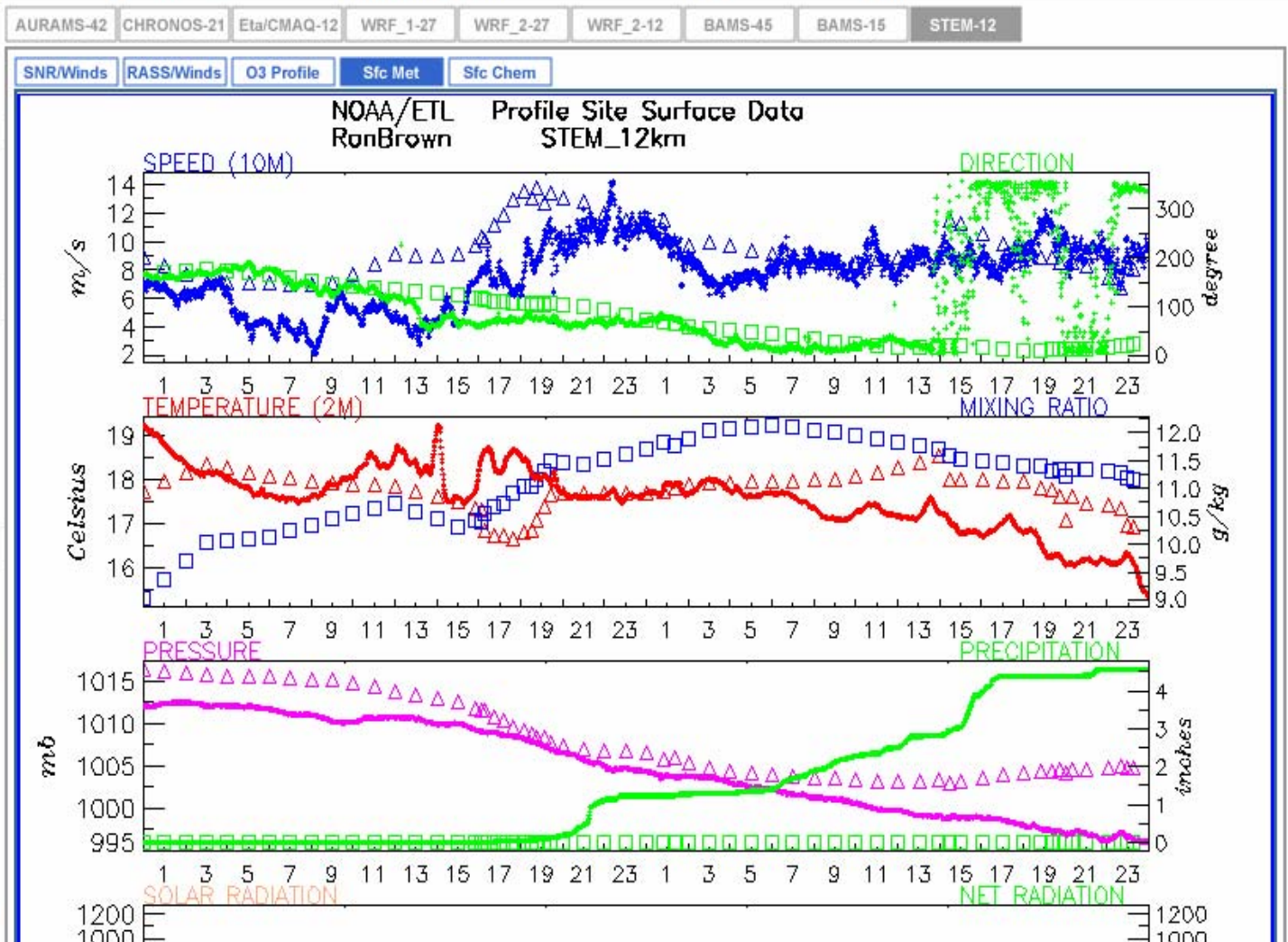
Ron Brown

**Data Archive**

Select a date:

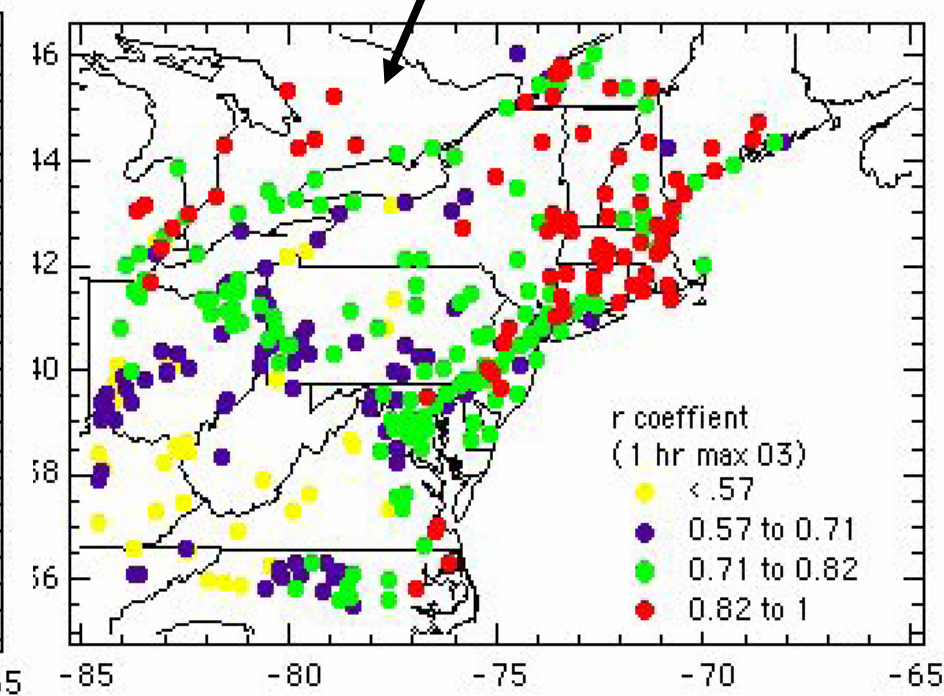
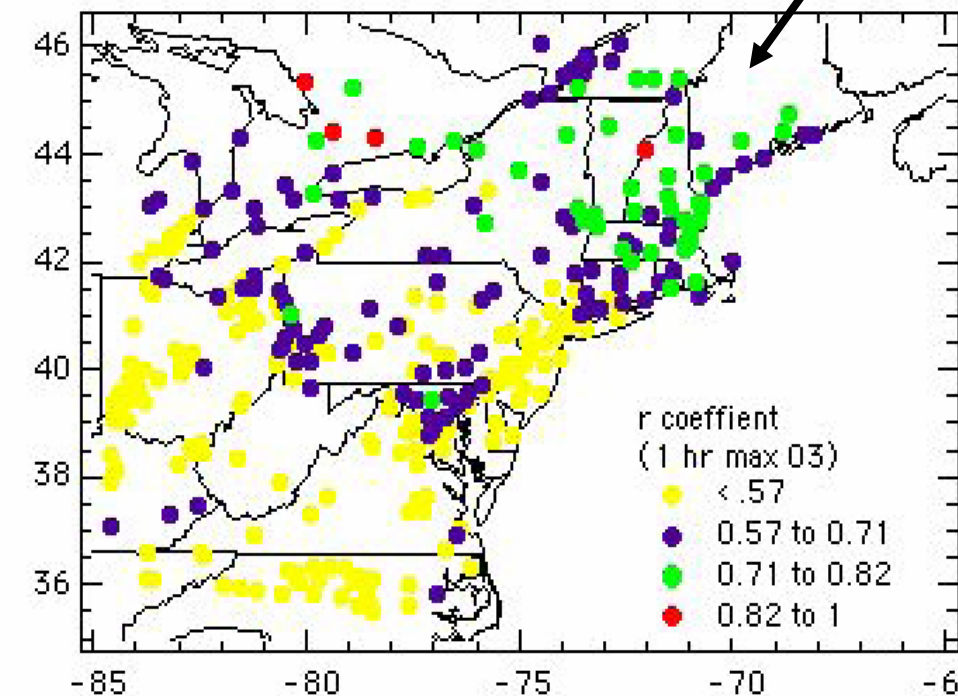
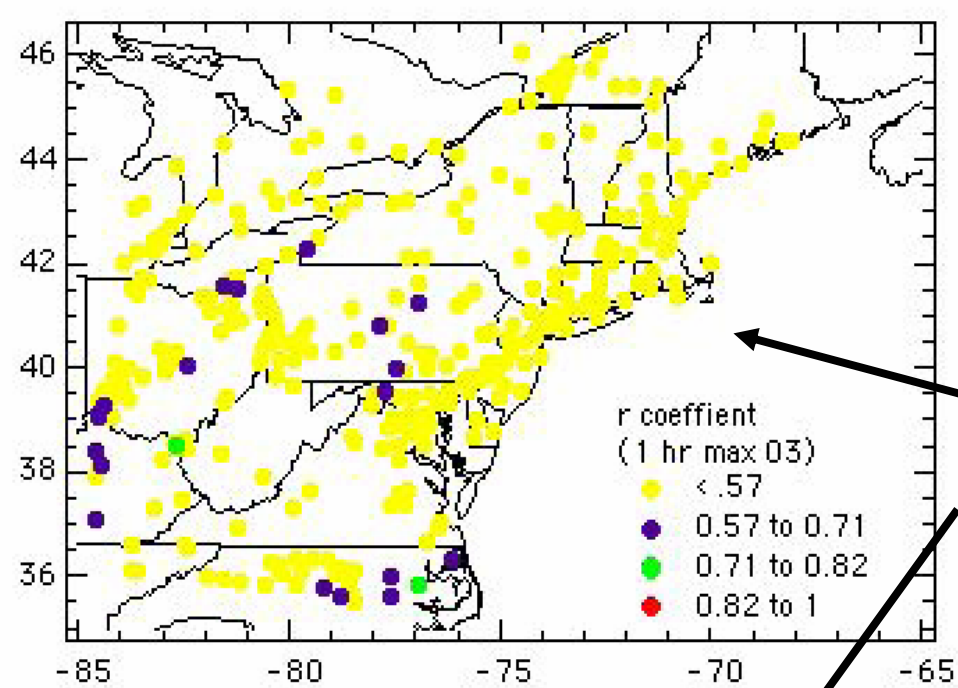
**July 2004**

Sun	Mon	Tue	Wed	Thu	Fri	Sat
				1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	31

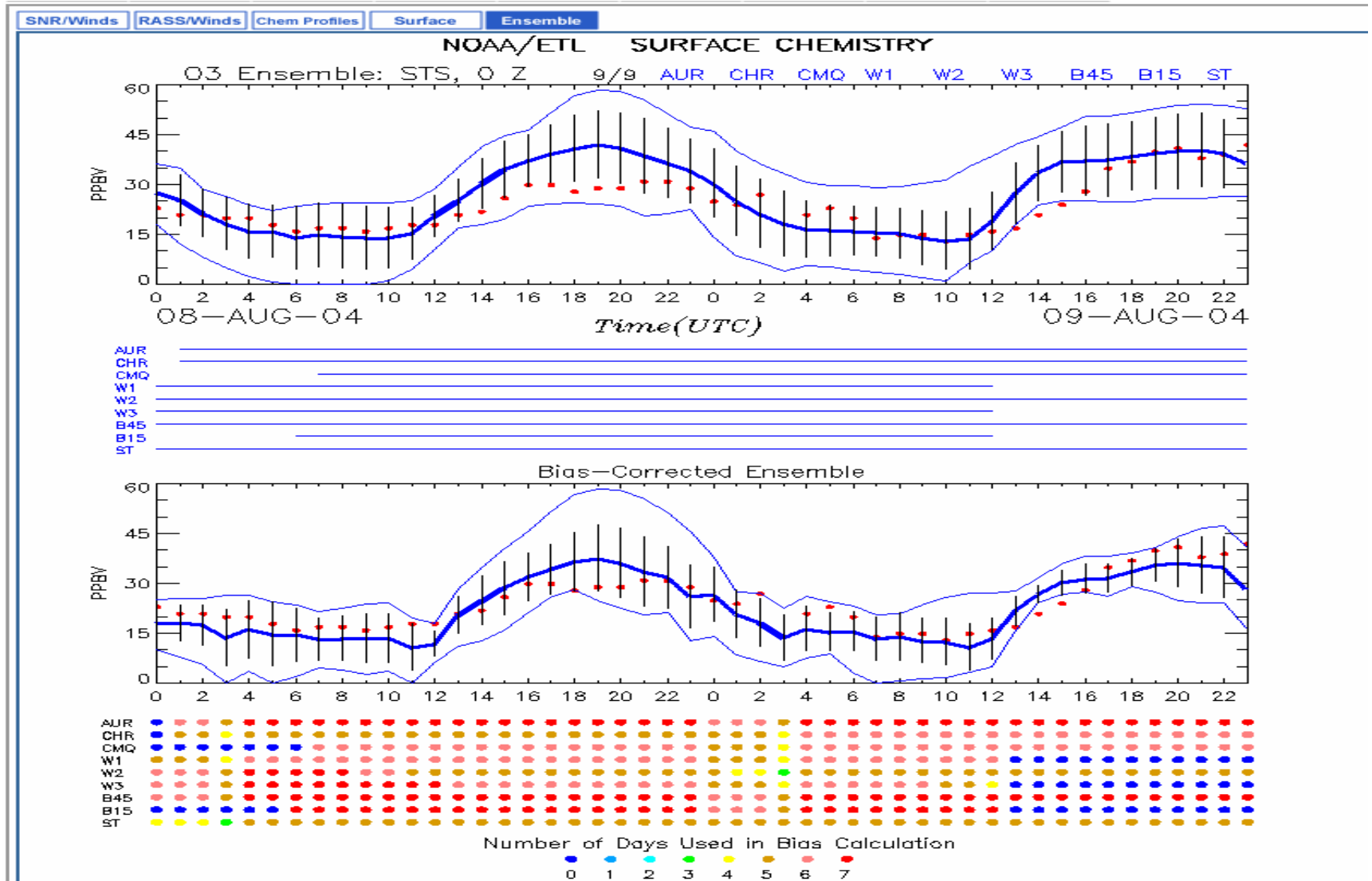


# Complimentary Actions to Improve Our Ability to Forecast Pollution are Needed

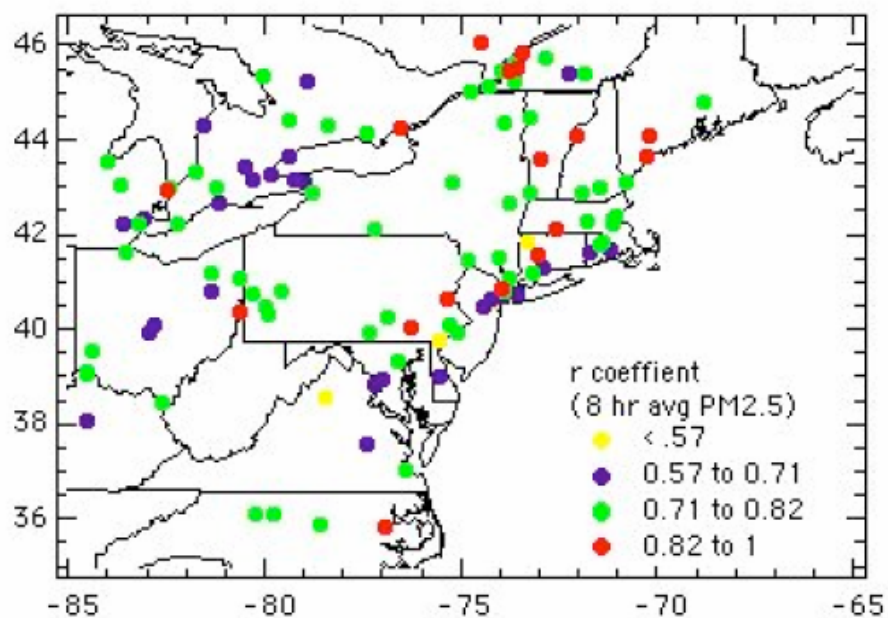
- \* Persistence
- \* Single Forward Model w/o assimilation
- \* Ensemble forecast (8 models) w/o assimilation



# Ensemble Techniques Help !



# Ensemble Methods Also Work for PM2.5 Forecasting



Comparison Statistics for Geometric Ensemble with AIRNOW daily 8-hr avg PM2.5 7/14/04 through 8/18/04

	median average	
r coeff.	0.75	0.73
Md/Ob ratio	0.86	1.00
ratio RMSE	1.76	1.90
Sdev	5.55	5.84
Skill factor (%)	= 75.42	

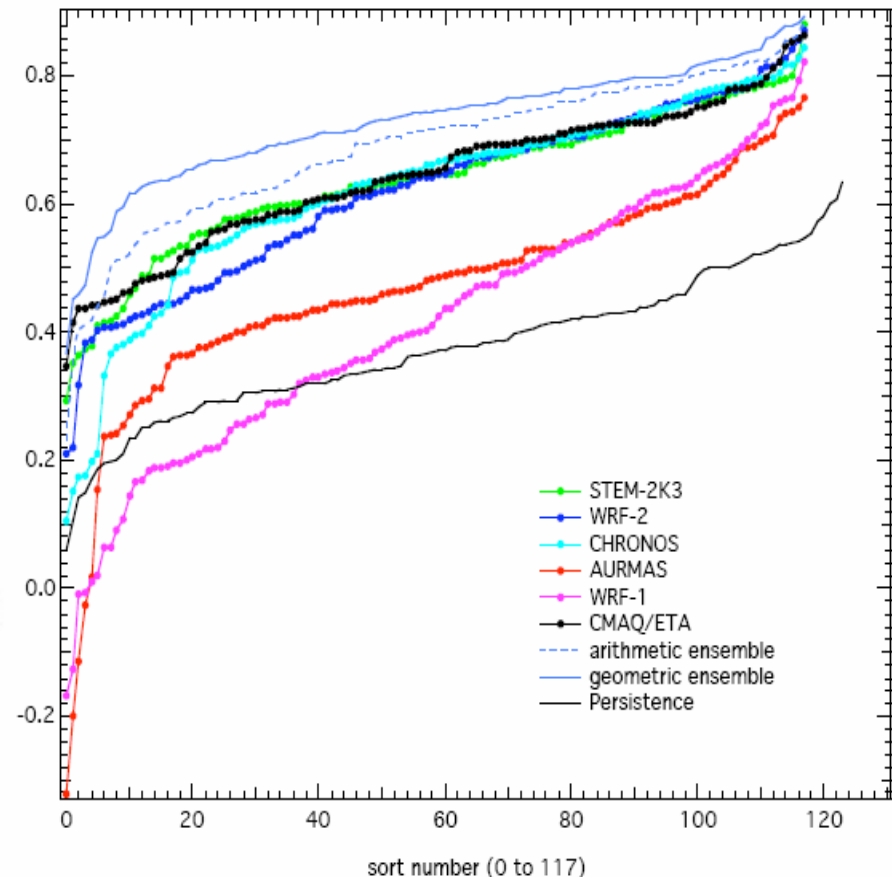
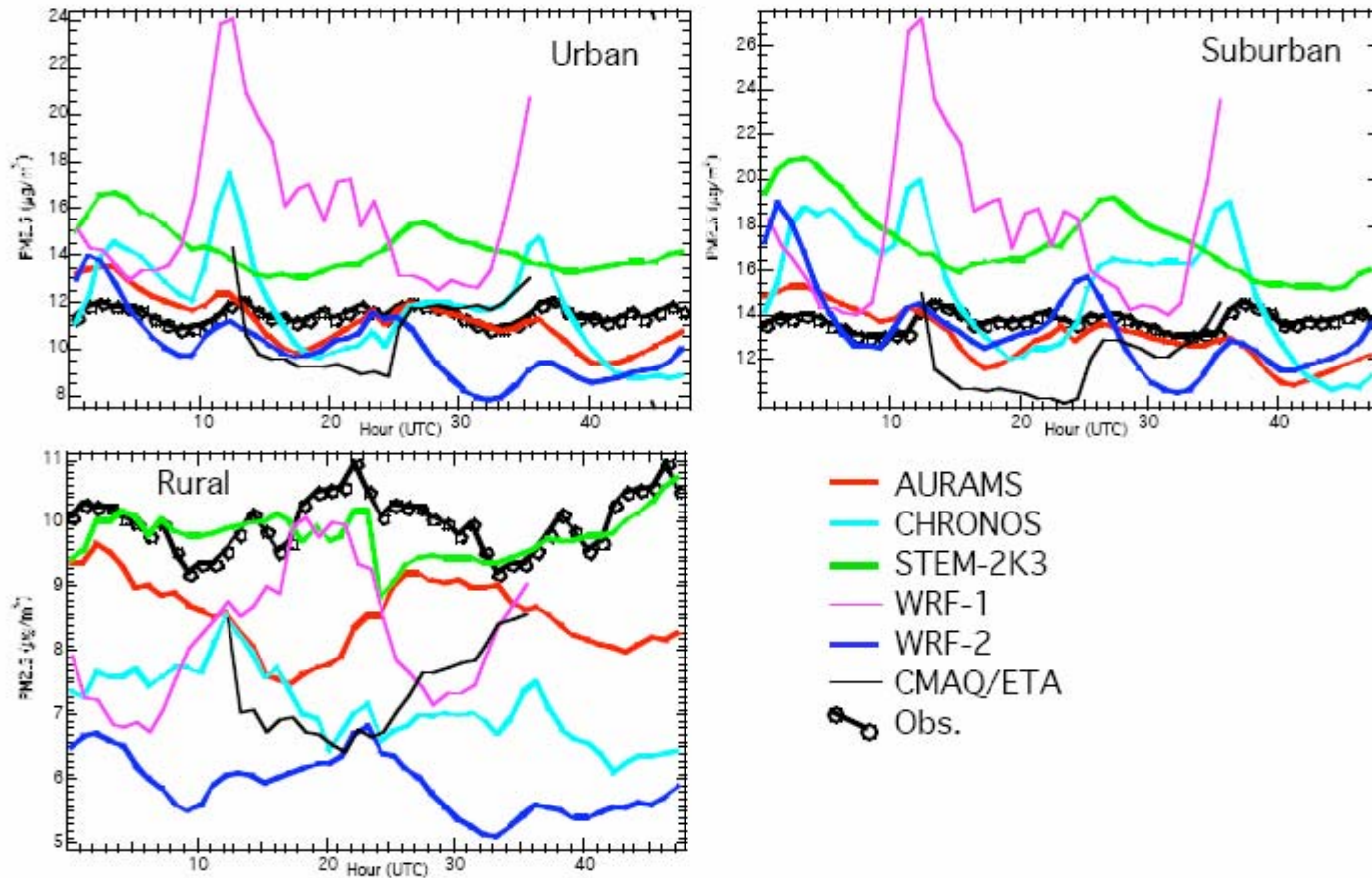


Figure 5. Sorted r-correlation coefficients for the 8 model cases, and persistence

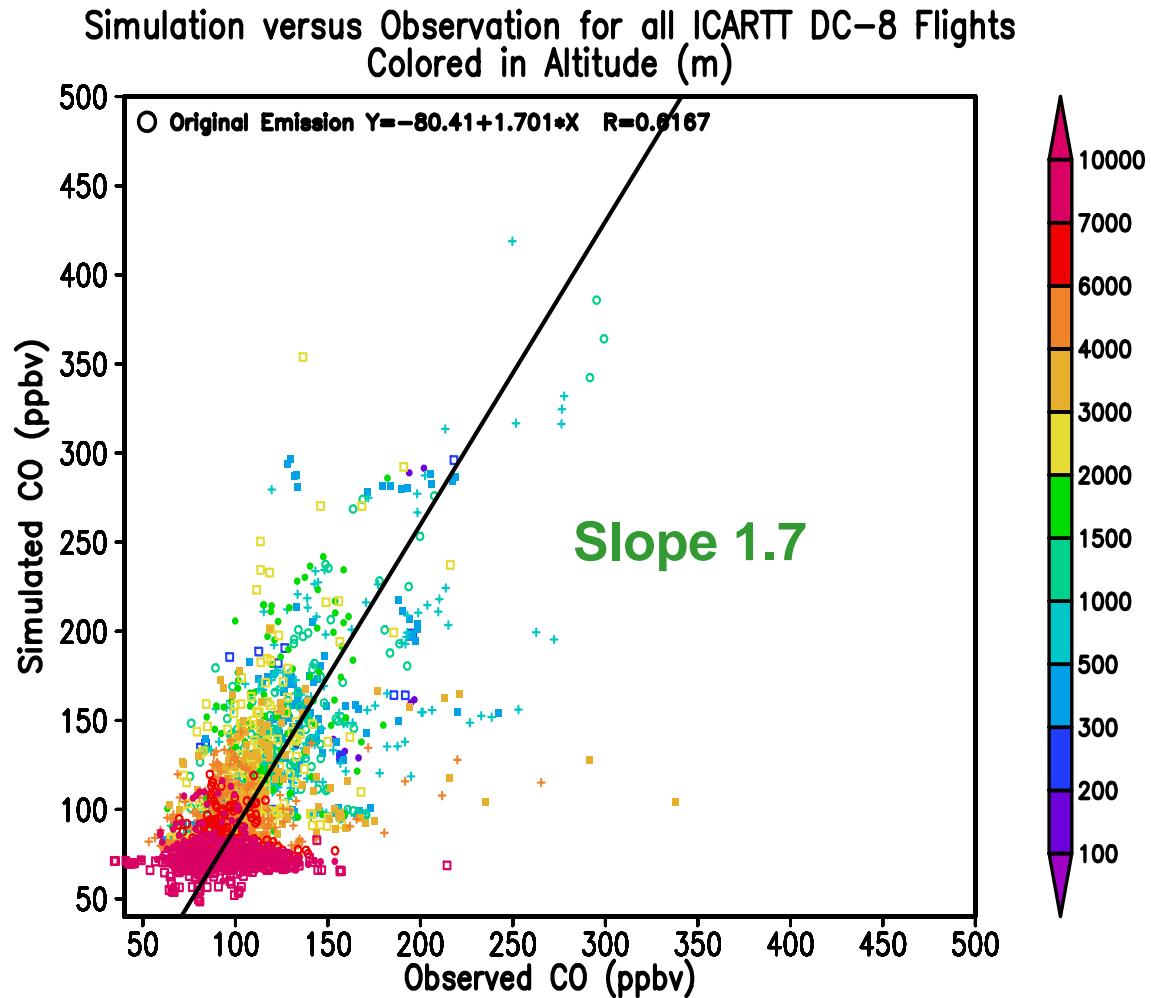
# But take little comfort..... We have a long way to go !!

PM2.5 Average Diurnal Profiles, summer 2004, in NE U.S.





# Emission Issues

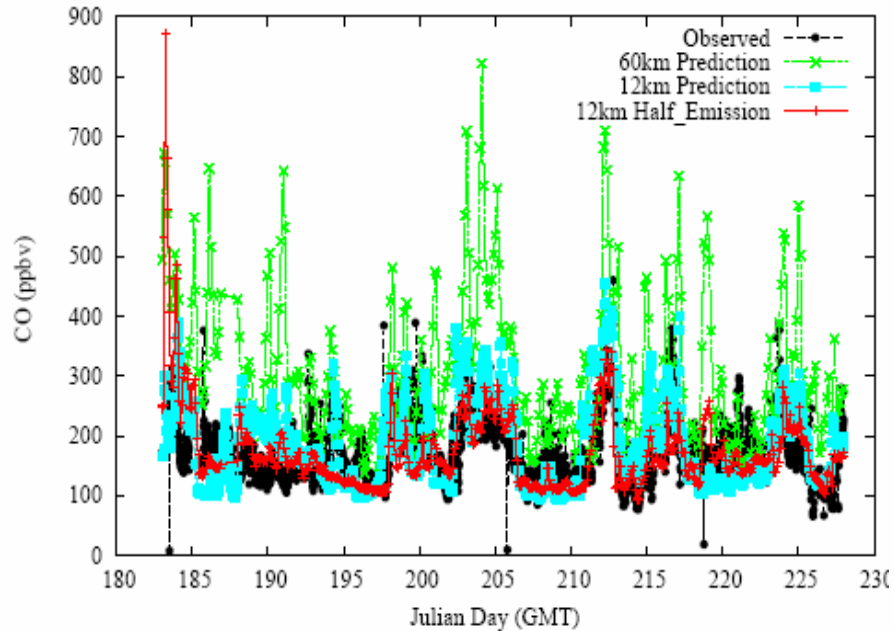


## Sensitivity Runs Using Reduced Emissions -- Correlations between STEM simulations and Measurements for All DC-8 flights

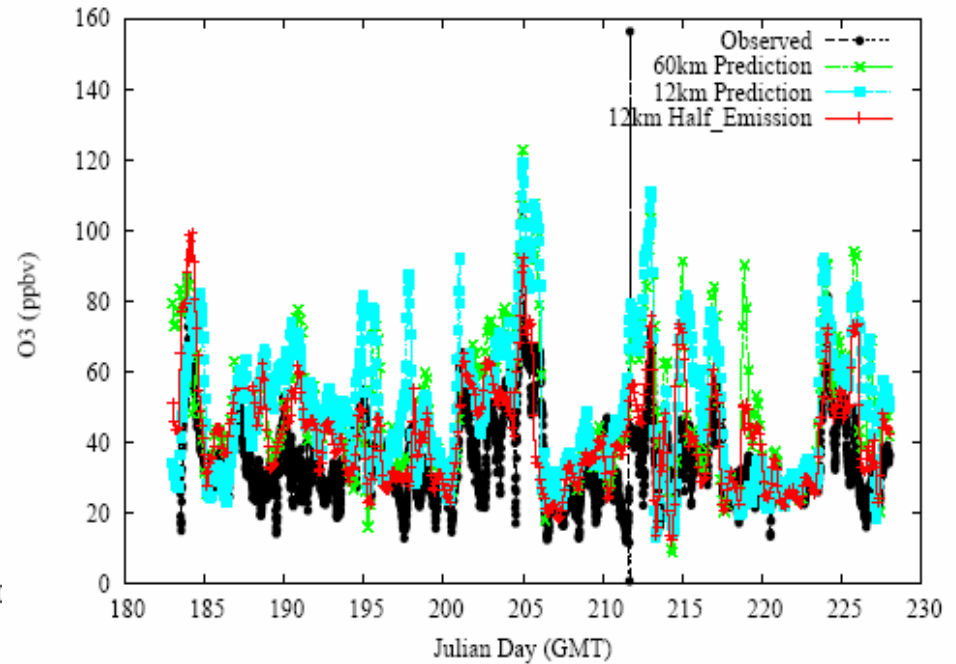
<b>Species</b>	<b>60 km simulation with original NEI-1999v3 emission</b>		<b>60 km simulation with half CO, NO<sub>x</sub> and SO<sub>2</sub> emissions</b>	
	Slope	R	Slope	R
<b>CO</b>	<b>1.70</b>	<b>0.62</b>	<b>0.83</b>	<b>0.66</b>
<b>NO<sub>y</sub></b>	<b>4.11</b>	<b>0.48</b>	<b>1.50</b>	<b>0.48</b>
<b>PILS SO<sub>4</sub><sup>2-</sup></b>	<b>2.52</b>	<b>0.75</b>	<b>0.78</b>	<b>0.75</b>
<b>SAGA SO<sub>4</sub><sup>2-</sup></b>	<b>3.06</b>	<b>0.74</b>	<b>1.13</b>	<b>0.74</b>
<b>PILS NH<sub>4</sub><sup>+</sup></b>	<b>0.35</b>	<b>0.35</b>	<b>0.33</b>	<b>0.48</b>
<b>SAGA NH<sub>4</sub><sup>+</sup></b>	<b>1.60</b>	<b>0.64</b>	<b>1.08</b>	<b>0.66</b>
<b>O<sub>3</sub></b>	<b>1.13</b>	<b>0.46</b>	<b>0.97</b>	<b>0.55</b>
<b>Ethyne</b>	<b>0.21</b>	<b>0.50</b>	<b>0.26</b>	<b>0.51</b>
<b>URI HCHO</b>	<b>0.82</b>	<b>0.84</b>	<b>0.89</b>	<b>0.84</b>
<b>H<sub>2</sub>O<sub>2</sub></b>	<b>0.56</b>	<b>0.70</b>	<b>0.47</b>	<b>0.67</b>

# Clear Improvement in Surface Predictions

Predicted and Observed CO (ppbv) over Isle of Shoals

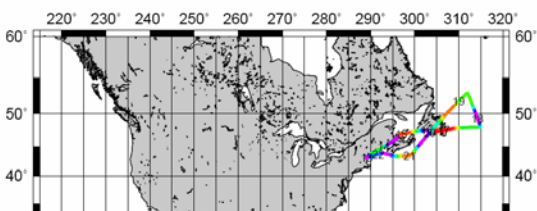
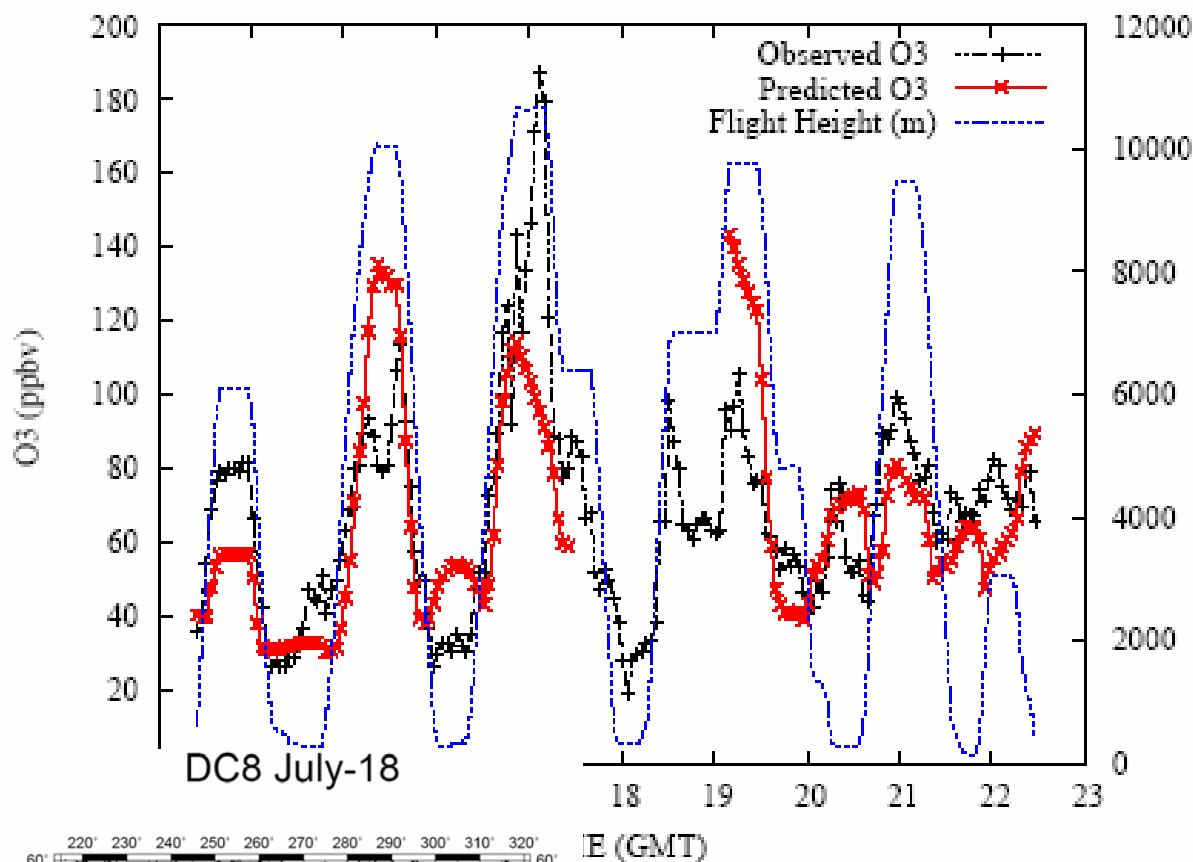


Predicted and Observed O3 (ppbv) over Castle Springs



# Integration of Measurements & Models

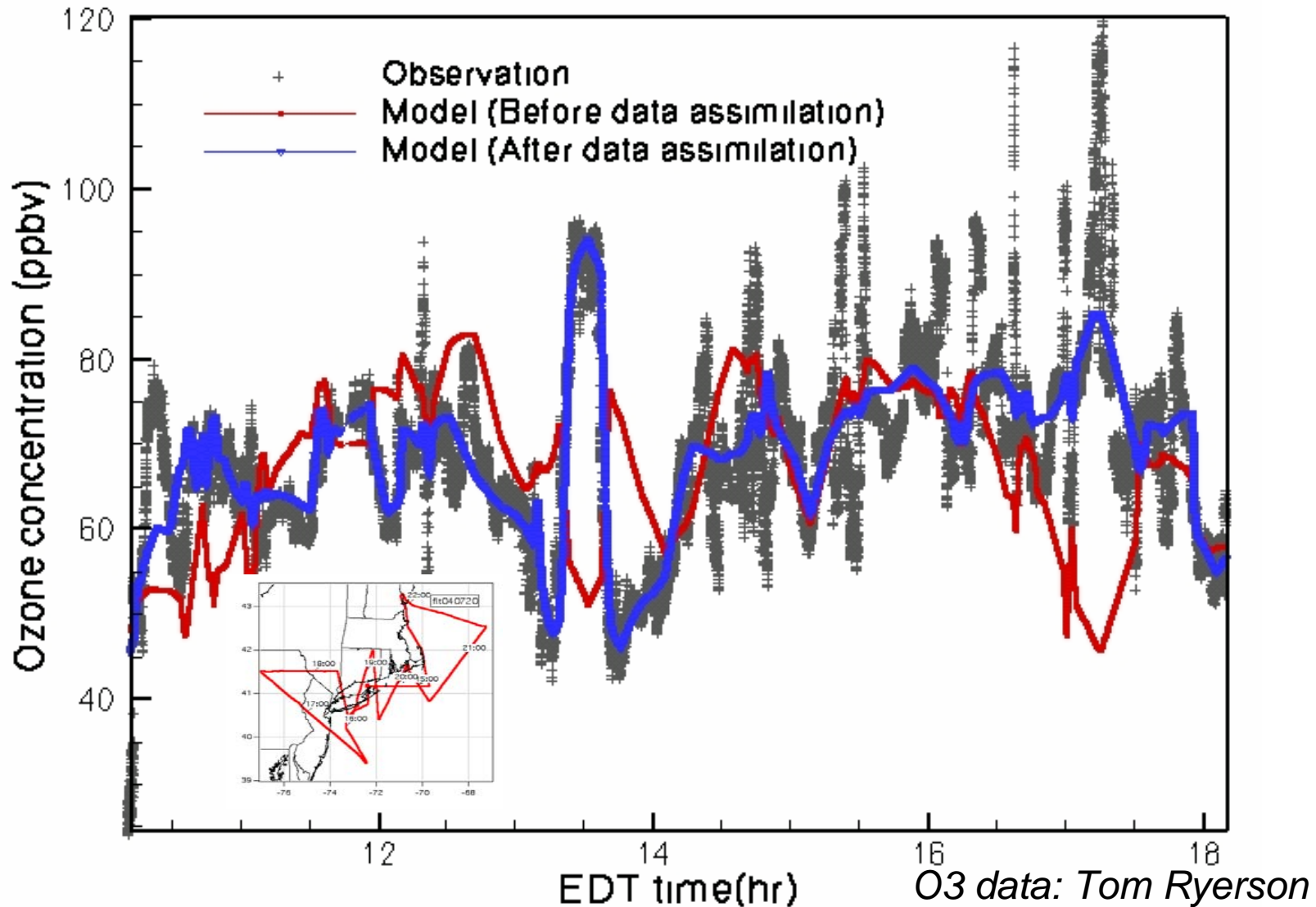
ICARTT DC-8 Flight #9 O<sub>3</sub> on 7/18/2004



Data: Larc

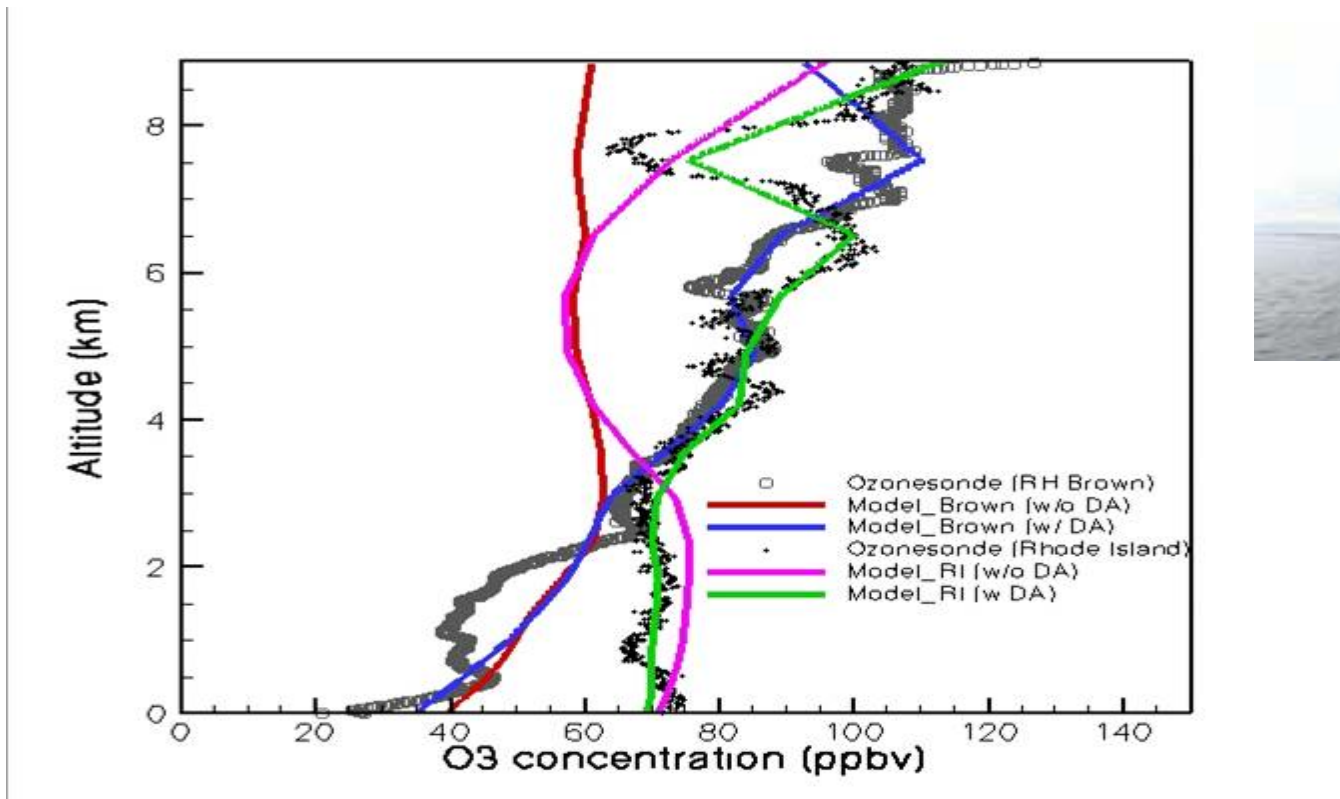
- **Cost functional** measures the model-observation gap.
- **Goal:** produce an **optimal state** of the atmosphere using:
  - **Model information** consistent with physics/chemistry represented
  - **Measurement information** consistent with reality
  - **within errors**

# Reanalysis of Ozone using Surface as Well as Ozone Profile and Aircraft Data



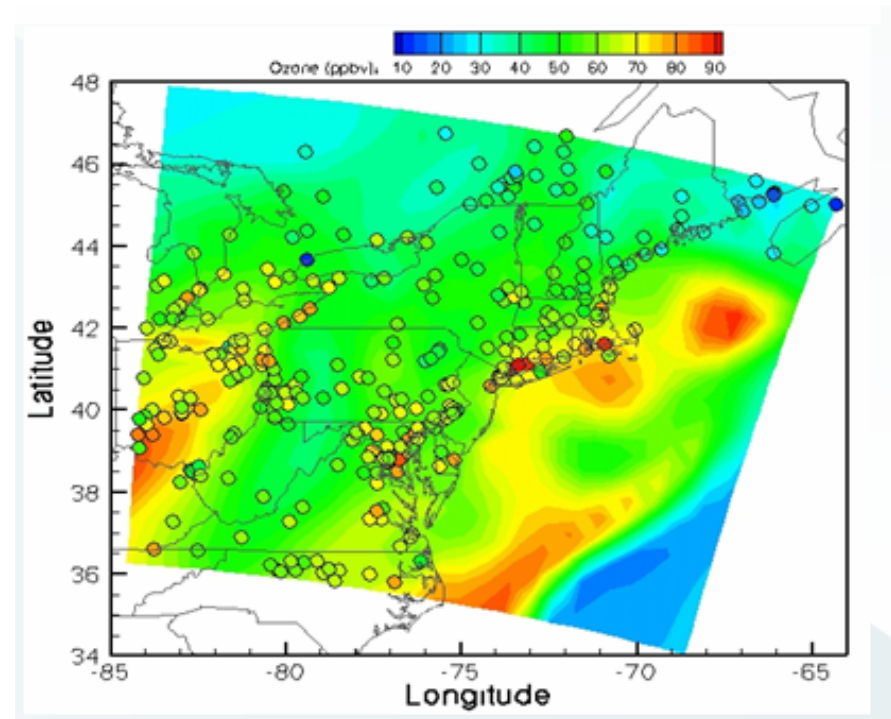
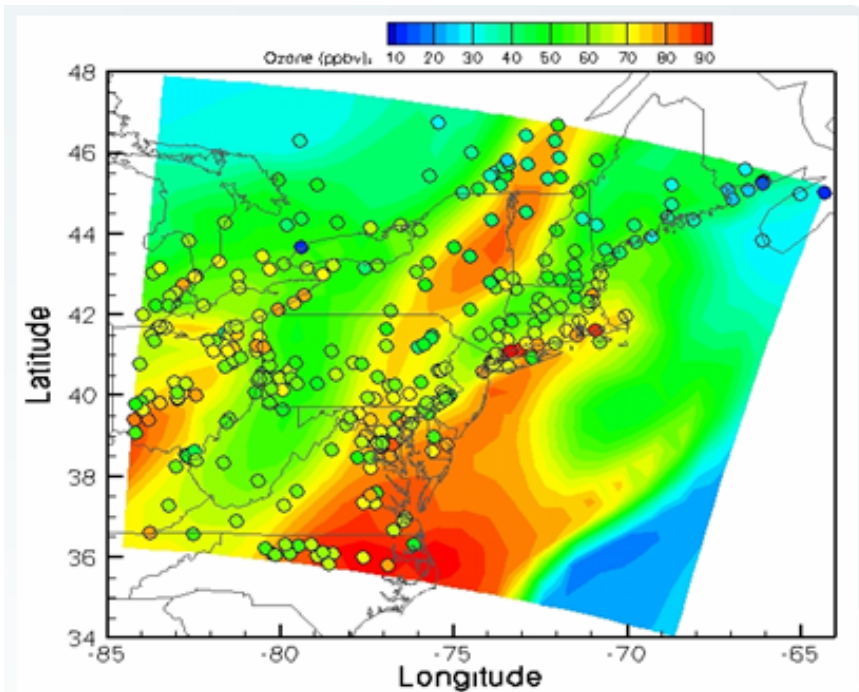
# Getting the Vertical Distributions Right is Critical

*Current models have a difficult time...so data  
assimilation is important*



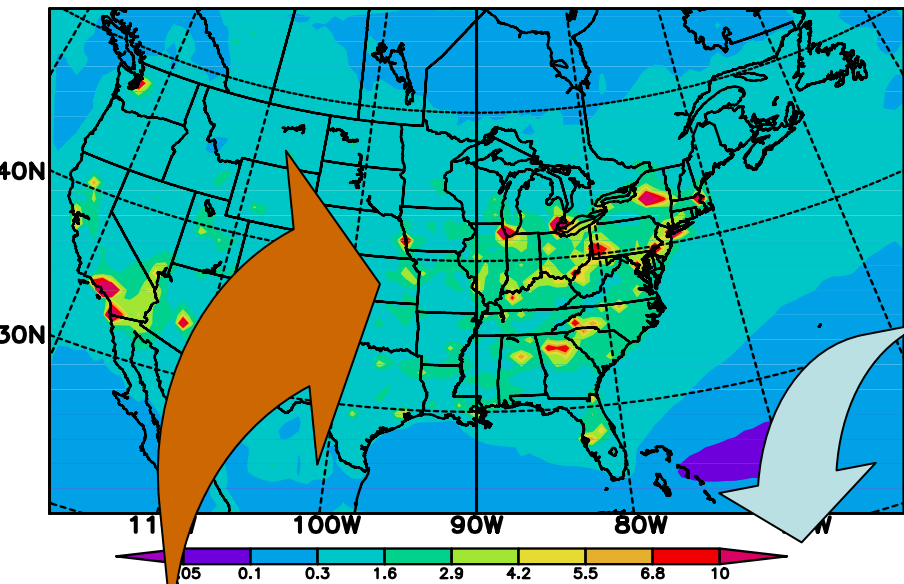
*IONS O3 data: Anne Thompson & John Merrill*

# Ozone Forecasts (*left*) and Reanalysis (*Right*)

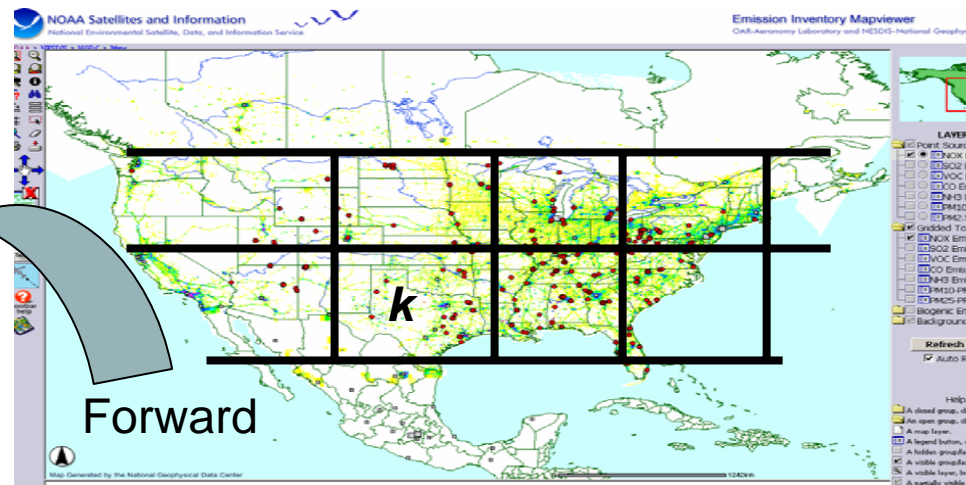


*Circles represent observations  
(locations and values)*

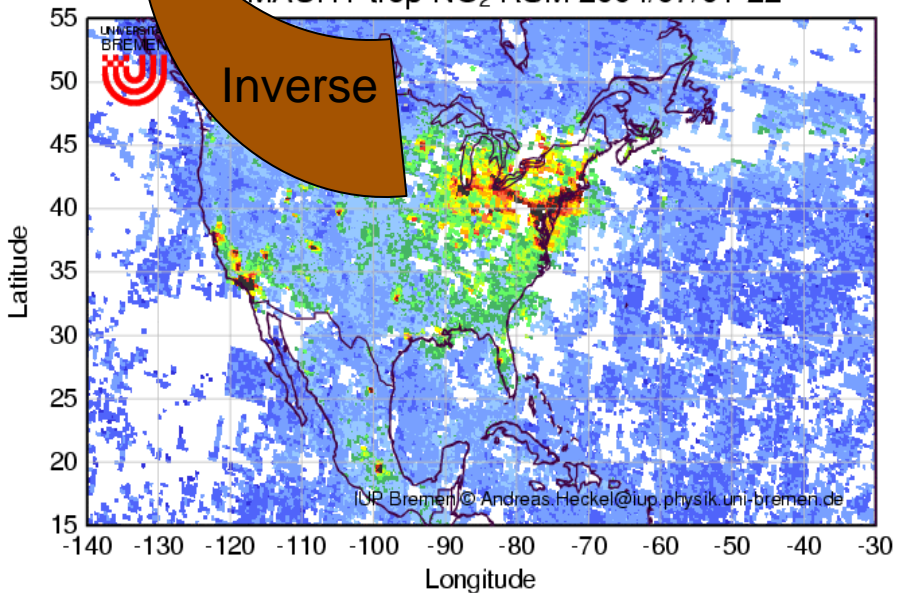
Monthly Averaged Forecasted NO<sub>2</sub> (10<sup>15</sup> molecules/cm<sup>2</sup>)



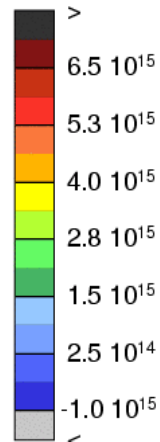
# 4dVar can be used to recover emissions



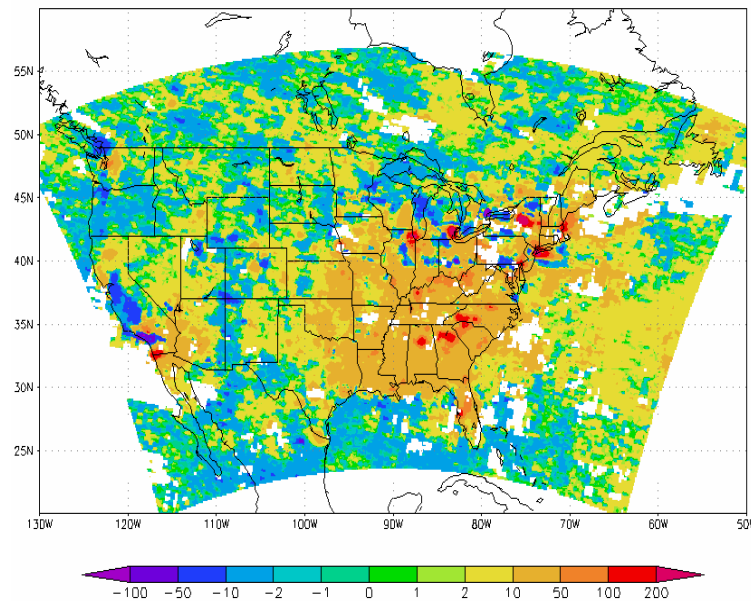
AMACHY trop NO<sub>2</sub> RSM 2004/07/01-22



VC NO<sub>2</sub>  
[molec cm<sup>-2</sup>]

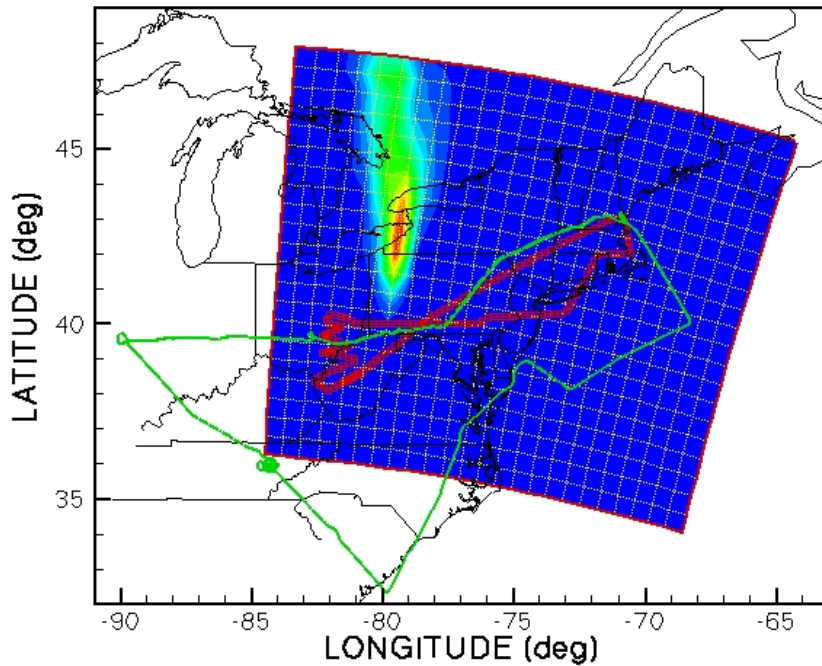


July Averaged NO<sub>2</sub> difference (Model-Obs) (10<sup>14</sup> Molecules/cm<sup>2</sup>)

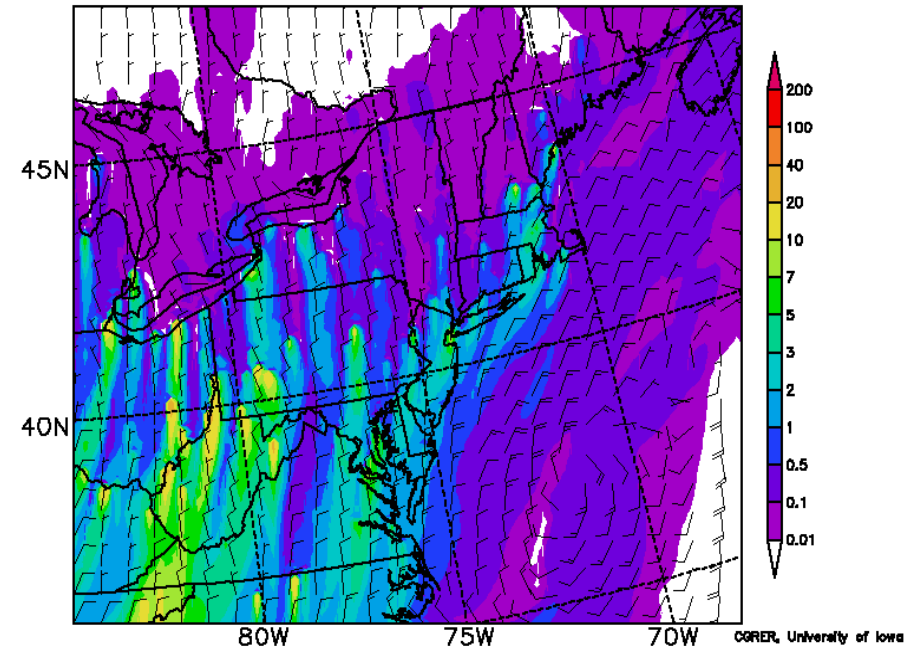




# Influence Function



Simulated SO<sub>2</sub> (ppbv) in the 400m layer  
at 21GMT, 08/06/2004



Adjoint Tools Can Also  
Help in the  
Characterization of  
Emissions

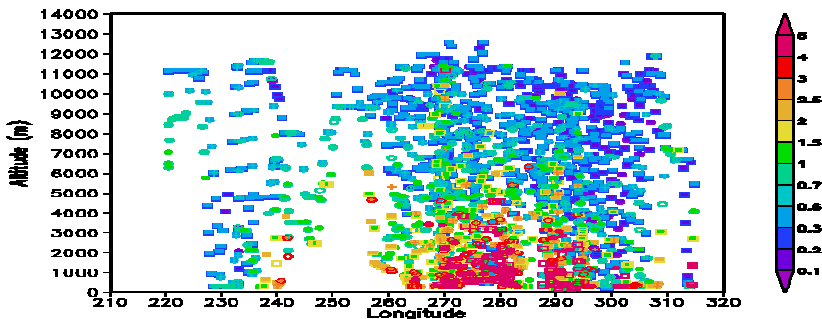
**Preliminary Results: CO  
emission scaling factor  
~ 0.7.**

# Regional Distributions of Aerosols

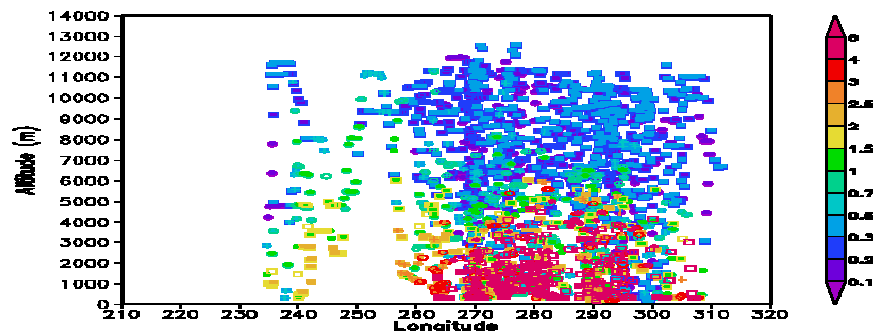
## Observed (PILS)

## Predicted

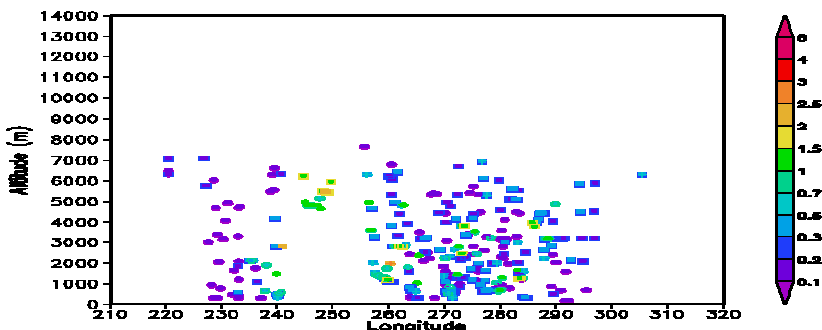
ICARTT DC-8 Flights colored in Observed Fine Sulfate ( $\mu\text{g}/\text{std m}^3$ )



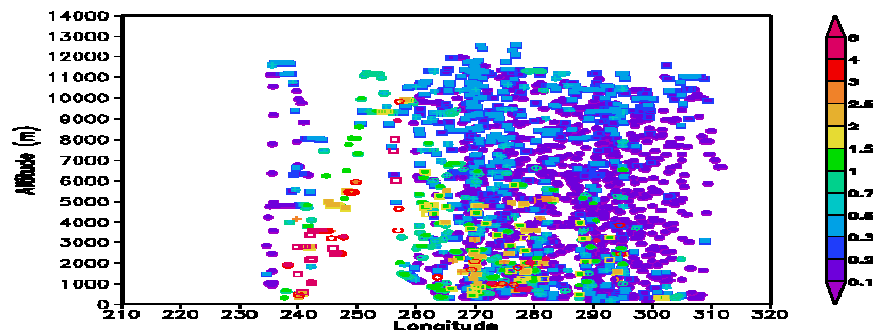
ICARTT DC-8 Flights colored in Simulated Fine Sulfate ( $\mu\text{g}/\text{std m}^3$ )



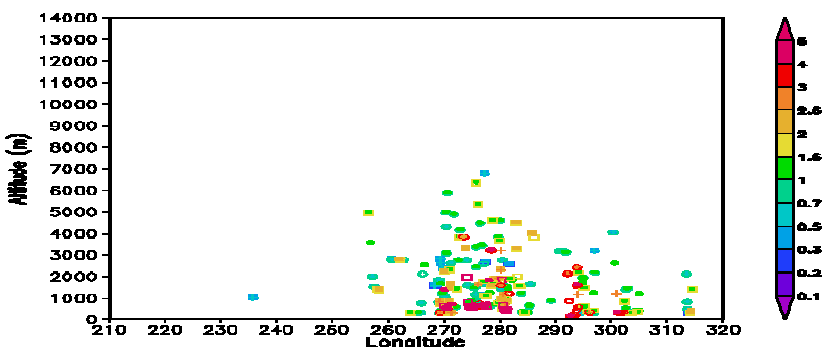
ICARTT DC-8 Flights colored in Observed Fine Nitrate ( $\mu\text{g}/\text{std m}^3$ )



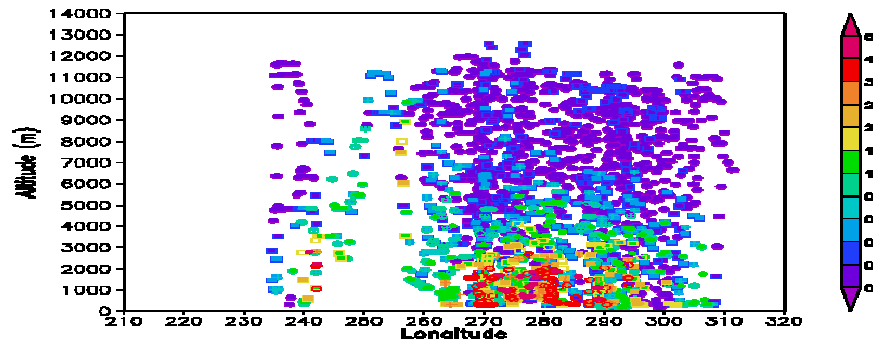
ICARTT DC-8 Flights colored in Simulated Fine Nitrate ( $\mu\text{g}/\text{std m}^3$ )



ICARTT DC-8 Flights colored in Observed Fine Ammonium ( $\mu\text{g}/\text{std m}^3$ )

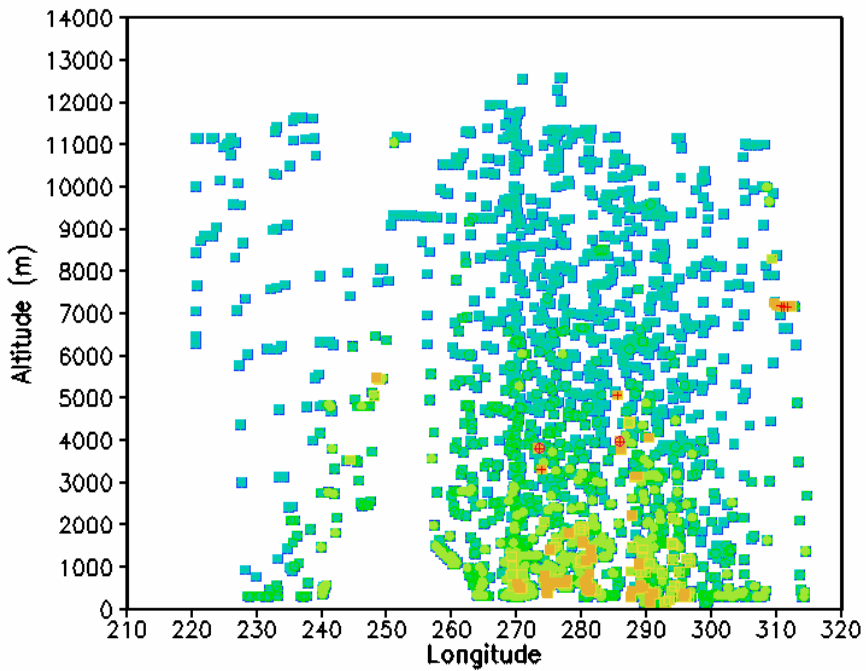


ICARTT DC-8 Flights colored in Simulated Fine Ammonium ( $\mu\text{g}/\text{std m}^3$ )

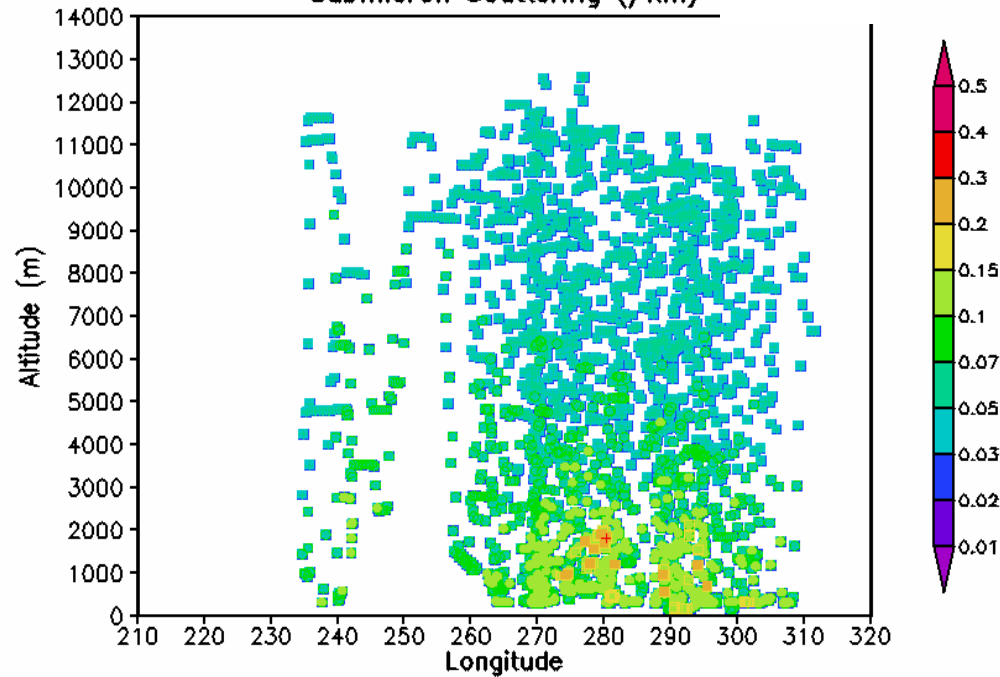


# Observed and Predicted Submicron Scattering

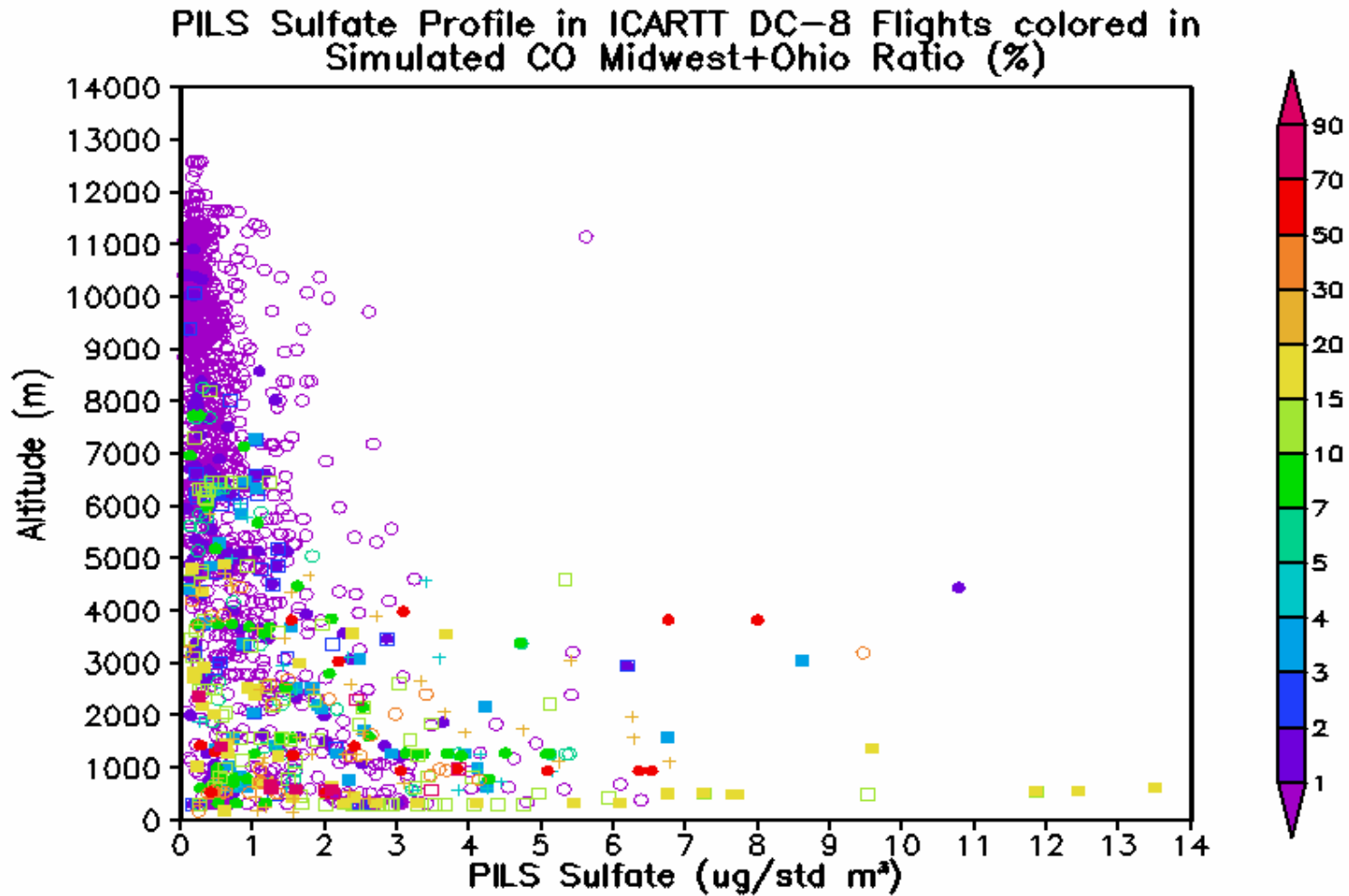
ICARTT DC-8 Flights colored in Observed Submicron Scattering



ICARTT DC-8 Flights colored in Simulated Submicron Scattering (/km)



# STEM Source Region Tracers Can Be Used to Sort Data & Complement Trajectories



# Future Plans

- Improve Base Emissions -- Update base year inventory (Streets and Vukovich), Biomass burning (others)
- Emission inversions
- Re-analysis using aircraft, surface, satellites, sondes (Ozone, CO, NO<sub>y</sub>, HCHO)
- Analysis of aerosols and optical properties, by better linking observations and models
- Better understand and constrain physical removal processes (dry and wet)

**We will submit our model products along the flight tracks**