Monitoring Needs for Improved Air Quality Modeling and Management in the Southeastern United States

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January 2002

Issue

- In the post-SAMI (VISTAS) world, what types of monitoring and measurements are desired to improve air quality modeling and management in the Southeast?
  - Measurement and monitoring needs for:
    - Air quality model development
    - Air quality model evaluation
    - Air quality management
  - Measurement vs. Monitoring
    - Monitoring is long term and consistent
- Perspectives from SAMI, FAQS and SOS modeling
  - SAMI: Regional focus
  - FAQS: State focus
  - SOS: Applied science focus

Considerations

- Monitoring
  - Routine monitoring of PM much more extensive now & in the future than for SAMI/SOS
    - Extensive mass monitors (almost useless for model evaluation)
    - States now have (limited) speciation of $PM_{2.5}$
  - Gas phase pollutant monitoring not significantly different
  - Satellite data will become available
- Emissions
  - SO_2 emissions will be lower
  - NO_x emissions likely lower
  - Most emissions estimates will remain highly uncertain
  - Little being done on speciation of organic PM
  - Little being done on size distributions
- Air quality
  - Urban ozone appears to be going down slowly
  - Possible increase in global transport of ozone and PM?
  - Sulfate likely to go down: OC likely to dominate PM2.5

Considerations (cont.)

- Meteorological Modeling
  - WRF will replace MM5 & Eta
    - Designed to go down to 1 km
    - Improved weather forecasting
      - Greater resolution and physics than Eta
- Air quality modeling
  - One-atmosphere modeling standard
    - CMAQ likely to be major player
    - Modeling domain will be ~continental
  - Major model component uncertainty will be PM dynamics
    - OC formation
- Major uncertainty in process still appears to be emissions

Emissions Inventory Assessment

Source	Emission scaling factor		
	August 1999	SAMI July 1995	SAMI May 1995
Total CO	1.01	1.08	1.26
Total SO_2	0.92	1.13	1.08
Area source NO_x	1.62	1.77	1.50
Elevated point source NO_x	1.48	1.31	1.24
Anthropogenic VOC	2.47	2.21	2.84
Biogenic VOC	1.11	1.24	1.17
Total NH_3	0.56	0.52	0.59
Total fine OC PM	1.10 (0.60)	0.49	0.62
Total fine EC PM	0.56	N/C	N/C

Using only IMPROVE measurements

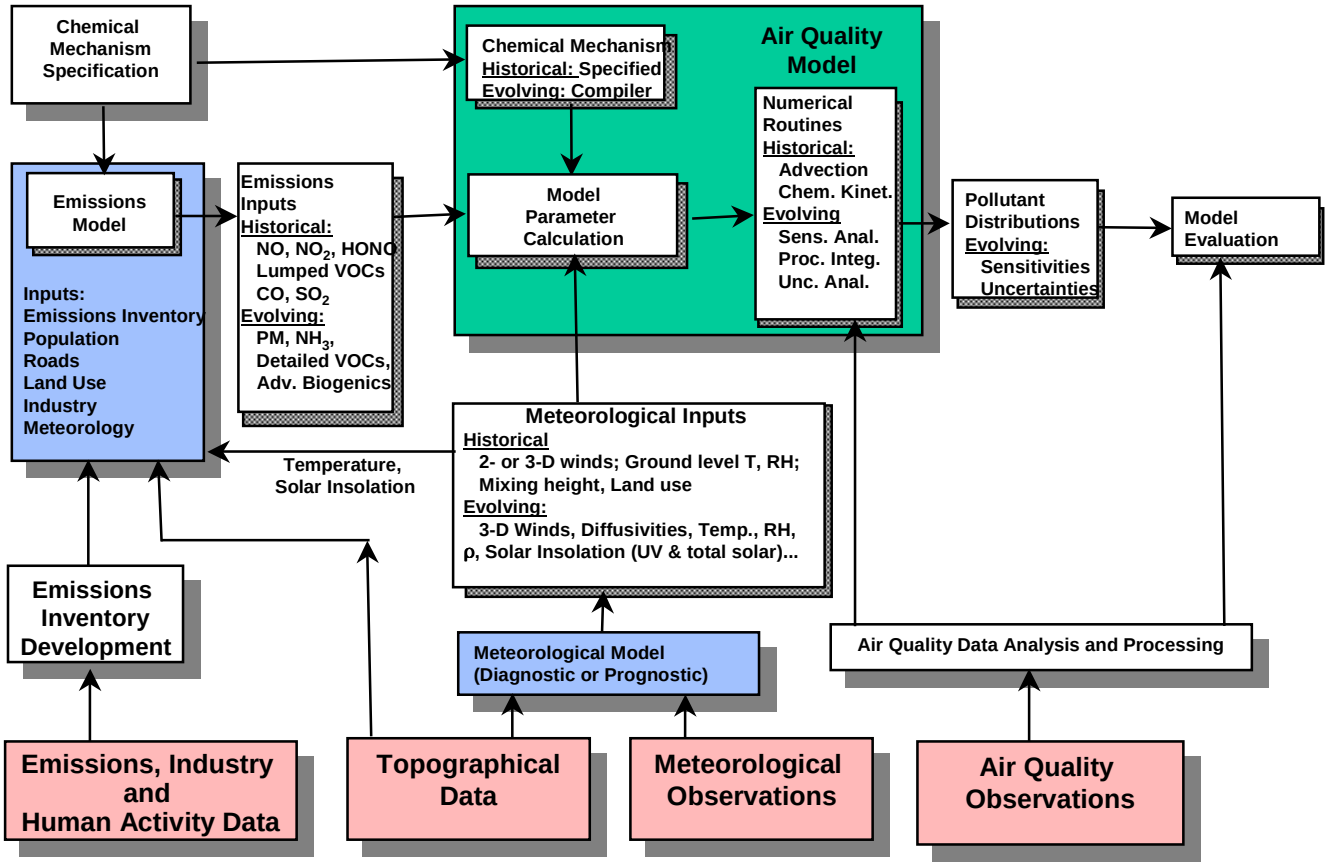
Confidence Levels in SAMI 1990 Base Year inventory

	Utility	Industry	Highway Vehicles	Nonroad Engines	Area
SO2	+++++	++++	+++	++	++
NOx	+++++	++++	+++	++	++
VOC	+++	+++	+++	++	++
NH3	+++	+++	++	+	+
PM2.5	+++	+++	++	+	+

Modeling Needs

- VISTAS will need to identify and model (at least) one year
  - Year should be representative (?)
- Model evaluation should be across a range of conditions
  - CMAQ still has not undergone “extensive” evaluation
  - Model development / improvements likely
- Good modeling requires lots of good data
  - Simulation accuracy
  - Model evaluation

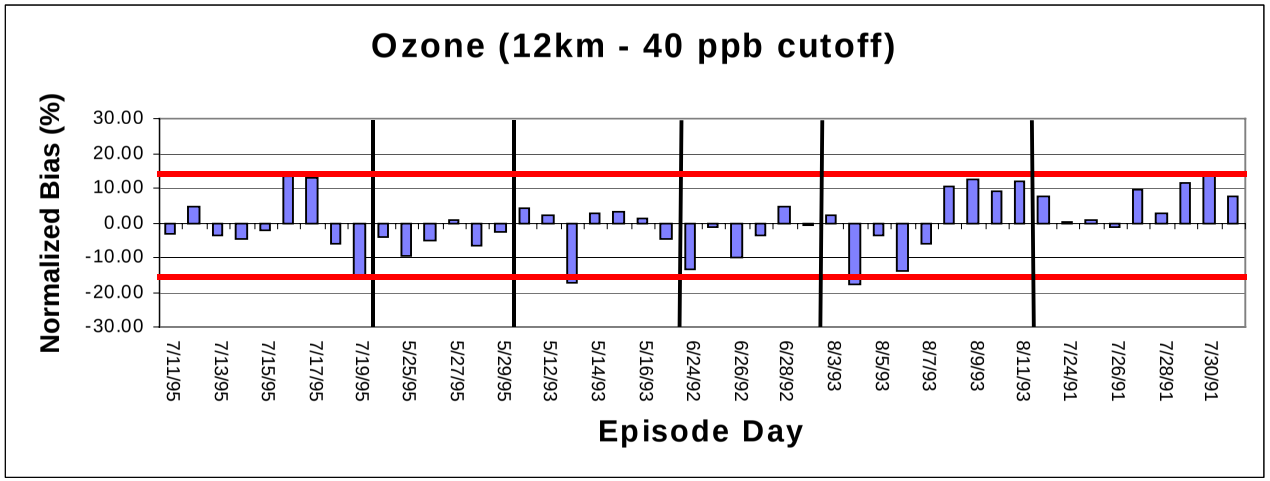
Modeling Process

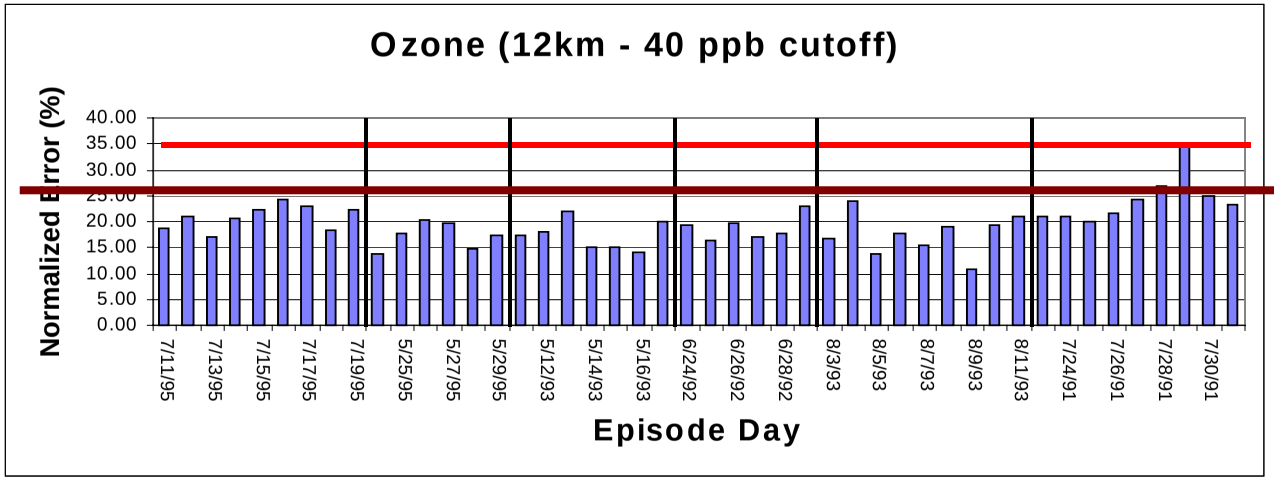


Personal Thoughts

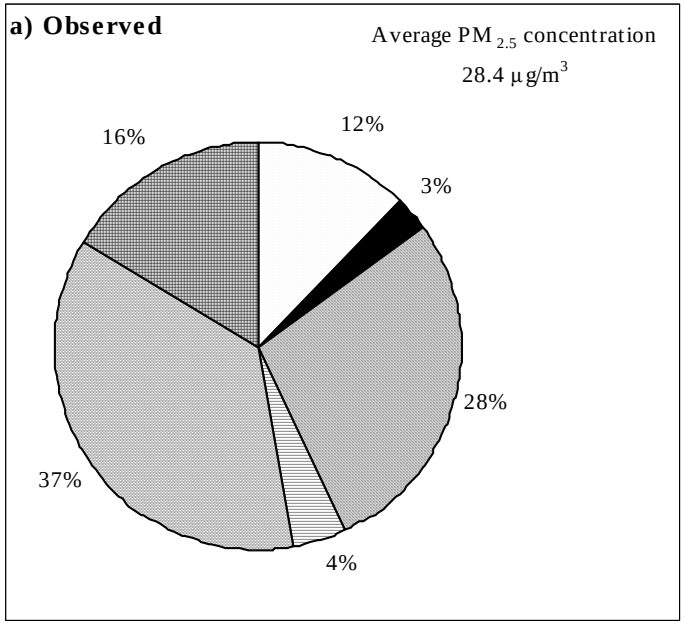
- Model simulations will never be perfect
  - Stochastic nature of atmosphere
  - Uncertainties / Errors in model inputs (met and air quality)
  - Model parameterization limitations
  - Thus, don't expect to be perfect, try to answer important questions
- Important questions
  - Can we explain the concentrations of pollutants at a location and time in terms of:
    - Source location and type
    - Processes impacting transport, formation and loss
  - Can we accurately estimate how pollutant concentrations will respond to controls
    - Can we show that we can do this?
  - Largest uncertainty: Source of organic and elemental carbon regionally

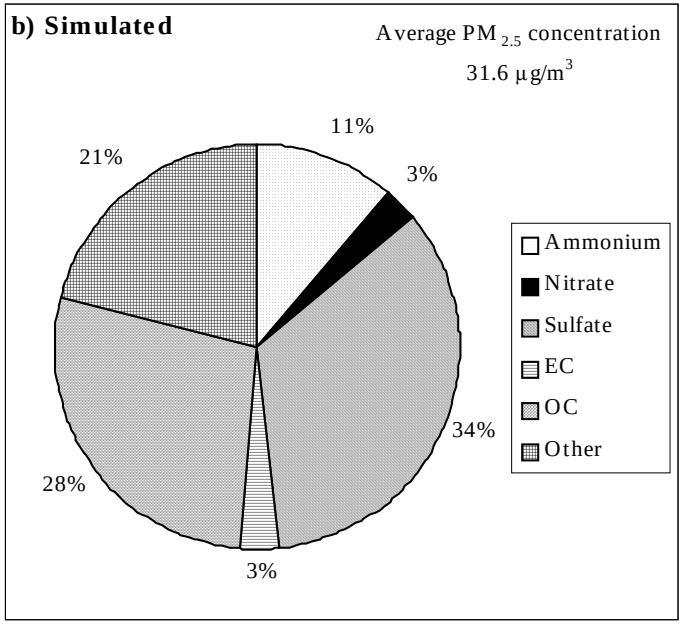
Model Uncertainty

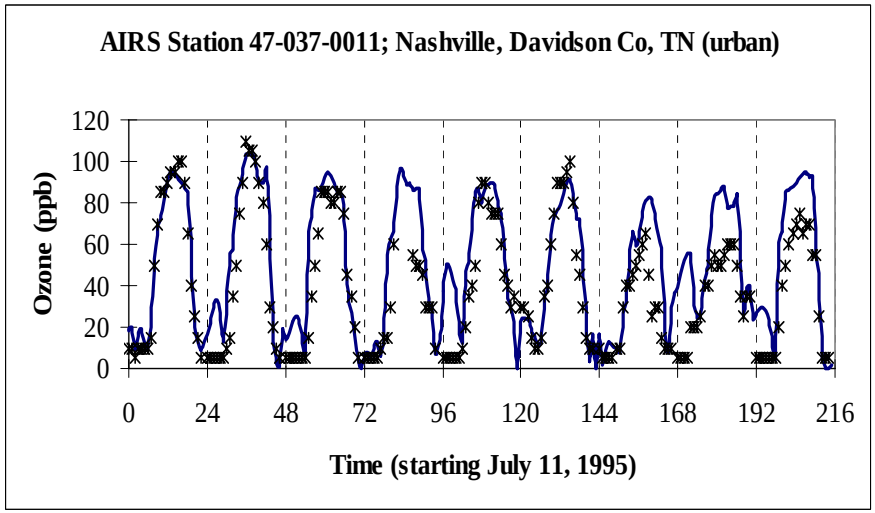


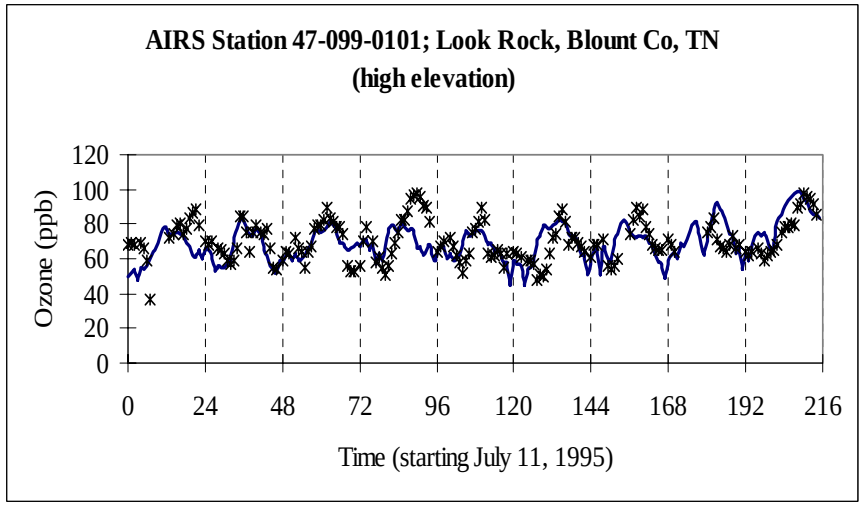


Limit due to sub-grid scale variation (point meas. vs. grid ave.):

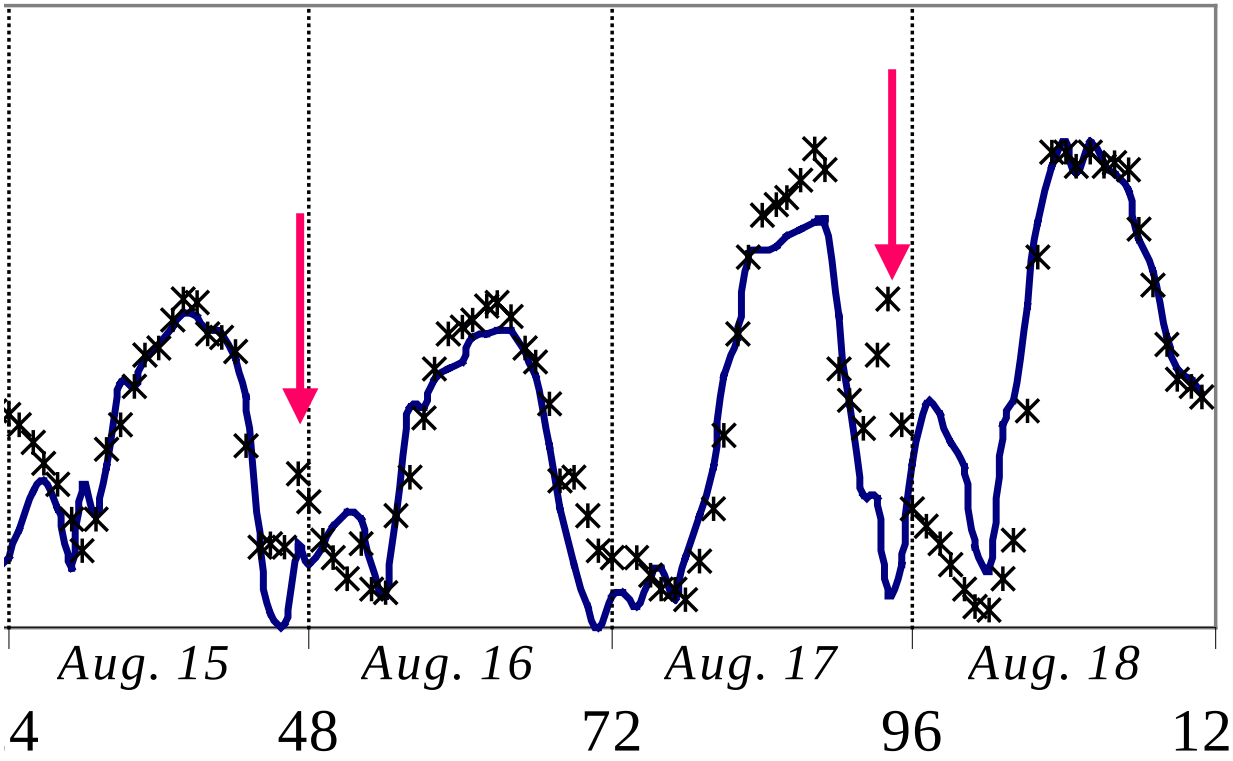

a) Observed
Average PM 2.5 concentration
28.4 µg/m3
12%
3%
28%
4%
37%
16%


b) Simulated
Average PM 2.5 concentration
31.6 µg/m3
11%
3%
34%
3%
28%
21%
Ammonium
Nitrate
Sulfate
EC
OC
Other


AIRS Station 47-037-0011; Nashville, Davidson Co, TN (urban)
Ozone (ppb)
0
20
40
60
80
100
120
0
24
48
72
96
120
144
168
192
216
Time (starting July 11, 1995)


AIRS Station 47-099-0101; Look Rock, Blount Co, TN
(high elevation)
Ozone (ppb)
0
20
40
60
80
100
120
0
24
48
72
96
120
144
168
192
216
Time (starting July 11, 1995)

Nighttime Bump (Macon, GA)



Balance between low inversion, turbulent mixing and fresh NO_x emissions

Key to Answering Question: Input and Model Evaluation

- Confidence in source-receptor relationships is developed by
  - Evaluating model inputs (both met and air quality)
  - Evaluating model outputs
  - Assessing uncertainties
  - Identifying problems
- Again, will never be perfectly confident

Monitoring Needs

- Monitoring needs are at a regional level
  - A few isolated, extra measurements will provide little benefit
    - For either meteorology or air quality
- Meteorological measurements
  - Temperature structure critical to met and AQ modeling
    - Appears to be less well simulated than other features
  - Rain (and snow)
    - Poorly simulated in models,
    - Point measurements not representative

Monitoring Needs (cont.)

- Major regional monitoring weaknesses:
  - Speciated $PM_{2.5}$ mass
    - Frequency of 24-hr
      - Should approach daily
    - More so: Continuous measurements very desirable
      - Can you imagine just checking to see how close a model predicts 24-hr average ozone?
      - Should move to add continuous capability at some sites
    - OC speciation
      - Can now speciate (some of) organic PM
        - » About the only way to explain / understand source of OC!!!
      - Should speciate organics for each season
  - Size distribution
    - Monitoring probably not necessary, but some characterization is.

Monitoring Needs (cont.)

- Regional monitoring needs (cont.)
  - Gas phase pollutants
    - Important for modeling PM!
      - Less emphasis now: could be a problem
    - Speciated organics
      - Needed to identify sources and evaluate model
        - » Ties in to speciated OC analysis
    - SO_2
      - Model sensitive to background (boundary) SO_2
      - Should monitor SO_2 in boundary states to characterize influx
    - Upper level
      - Some sensitivity to upper level concentrations, largely unknown
      - Some measurements of upper level gas-phase pollutants useful

Air Quality Measurement Needs

- CMAQ still in need of detailed evaluation
  - Likely developments and improvements
    - Requires detailed measurements
  - Most detailed measurements during summer
    - PM is an annual problem, and some components higher / dominate in winter (OC / EC)
  - Need detailed winter study?
    - ESP02 may provide needed data set for model testing
    - ESP01 probably will provide solid data set of summer CMAQ testing
      - Meteorology was a bit uncooperative
  - Not apparent what intensive measurements are needed until we see what is available from ESP01 and ESP02.

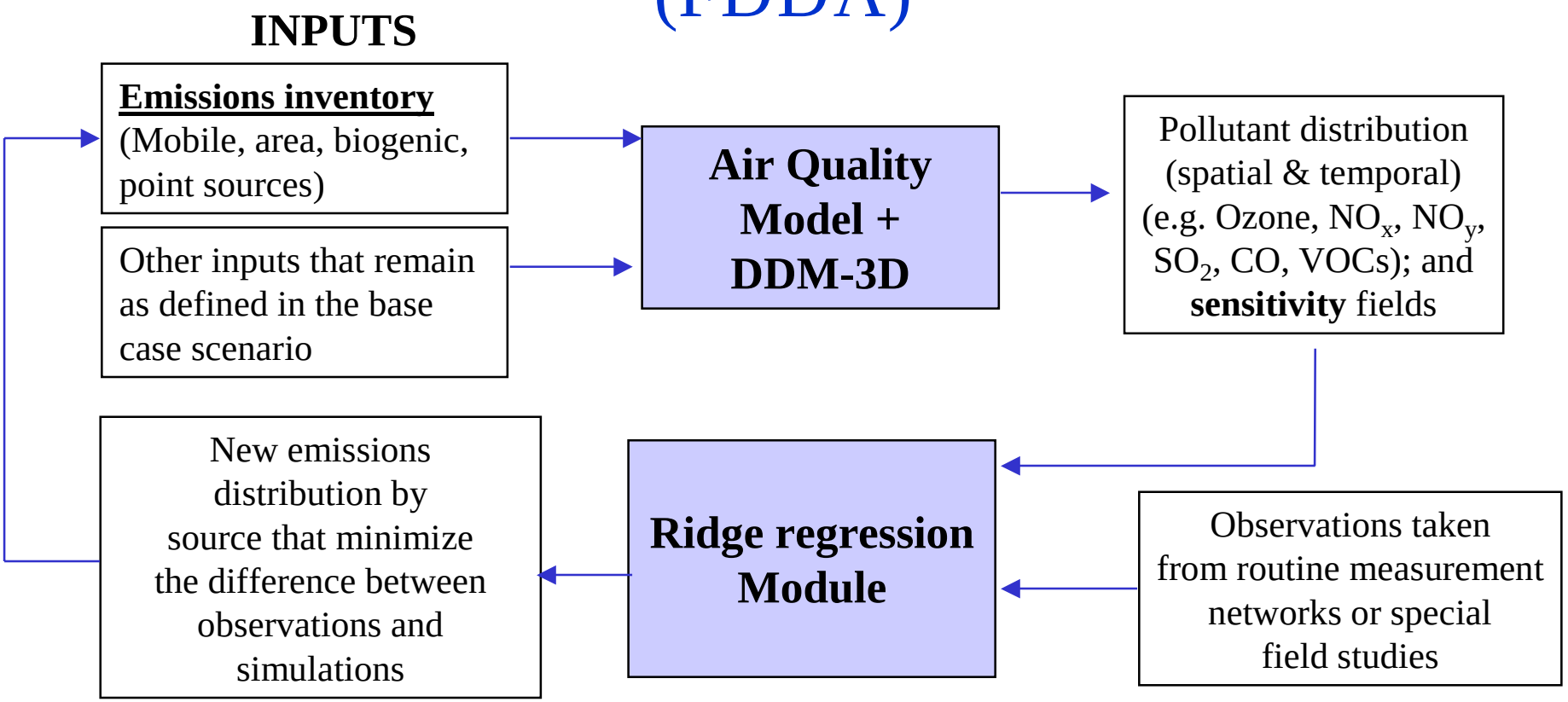
Emissions Measurement Needs

- Driving considerations
  - Greatest uncertainties due to emissions
  - OC will be of increasing importance
    - Reductions in sulfate
    - Health impacts (?)
  - Increased ammonia, lower SO2 can lead to increased nitrate
    - LA example
- Greatest needs
  - Understanding OC PM and precursor emissions
    - Ability to rectify sources difficult
      - Highly uncertain emissions
      - Model parameterizations uncertain
    - Measure OC composition of major sources
      - Mobile, wood burning, biogenic…
  - Ammonia emissions uncertainties
    - Design study to better characterize ammonia emissions from major sources (soils, mobile, confined feeding…)

Measurement and Monitoring Priorities

- Air quality model development
  - Detailed measurements needed
  - Monitoring useful to identify problems as well
- Air quality model evaluation
  - Consistent monitoring needed
  - Some additional measurements desirable
- Air quality management
  - Long term monitoring of most value

Emissions Inventory Assessment using Four Dimensional Data Assimilation (FDDA)



Main assumption in the formulation:

A driving source for the discrepancy between predictions and observations is the emission estimates

Estimated emission adjustments for domain-wide emissions from FDDA

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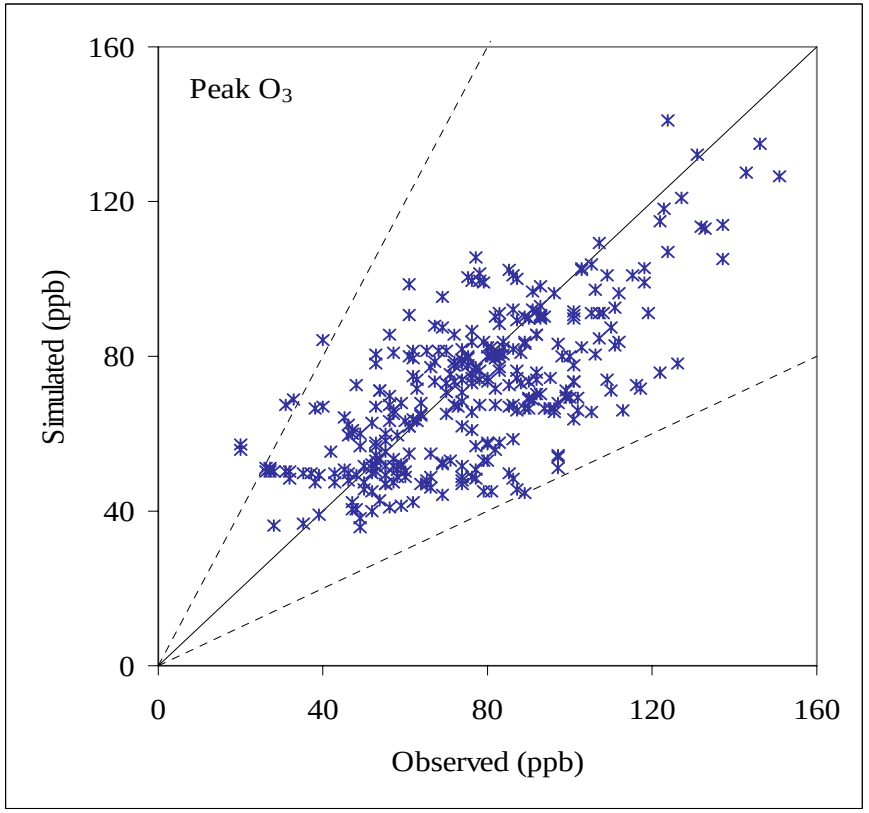
* Includes mobile and area sources

Ozone: Simulated vs. Observed

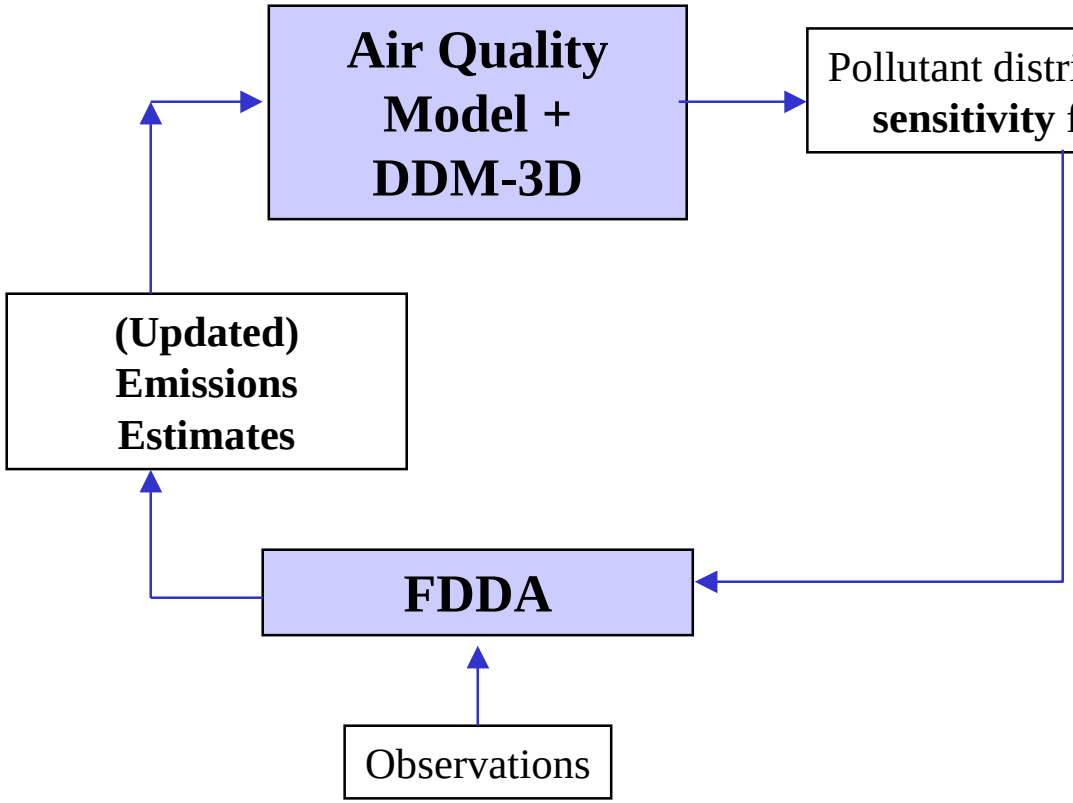
Peak Ozone



Pearl River Delta Application

- Current concern about source of air pollutants in Pearl River Delta Area
  - Emissions highly uncertain
  - Limited analysis to date (but not zero… see work by Zhang and co-workers)
- Apply DDM-3D and FDDA
  - Source apportionment using DDM-3D similar to SAMI
    - Identify source regions and contributions
  - FDDA to continue to improve emissions estimates
    - Evolutionary improvement of emissions

Evolutionary Improvement of Emissions Estimates and Source Impact Analysis



Emissions estimates improve with each application as more observations are assimilated and additional emissions studies are conducted: valuable information generated each application

Conclusions

- Developed a “one atmosphere” air quality model
  - Ambient gas and aerosol concentrations
  - Pollutant deposition
  - Sensitivity Analysis
- Applying to the eastern United States
  - Class I areas of the Southern Appalachian Mountains
  - Northeast & Southeast
- Evaluated results against monitoring databases
  - More details at http://environmental.gatech.edu/SAMI
- Simulating future air quality to determine the most effective emission control strategies
- Developed FDDA-based emissions analysis approach
- Foundation for other studies
  - Economic analysis of control
  - Area of influence
  - Pearl River Delta Area: evolutionary improvement of source impact assessment and emissions estimates