



GEORGIA
DEPARTMENT OF NATURAL RESOURCES

ENVIRONMENTAL PROTECTION DIVISION

Photochemical Grid Modeling 101

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Lexington, KY
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OUTLINE

- Background
- Model Inputs
- How the Models Work
- Model Performance Evaluations
- Probing Tools
- Computer Resources
- Personnel
- IT Support
- Example Applications



BACKGROUND





TYPES OF AIR QUALITY MODELS

- Steady-State Plume Model

- AERMOD

- Lagrangian Puff Model

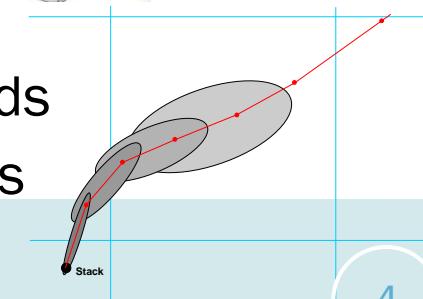
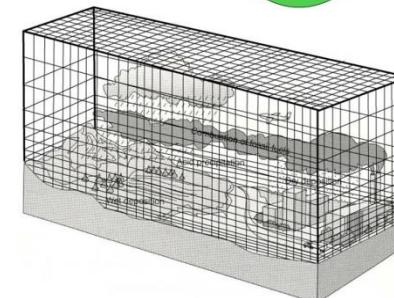
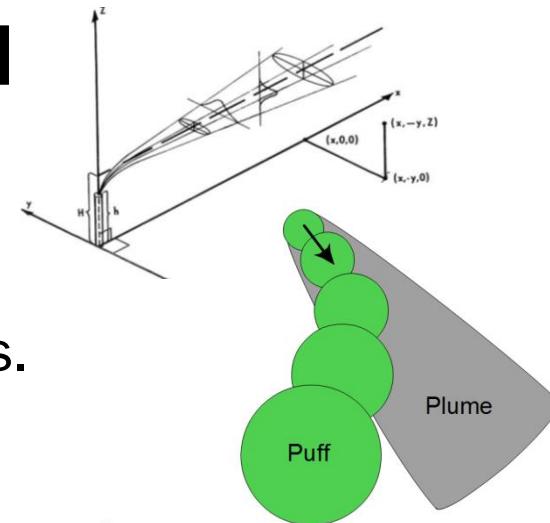
- Coordinate system follows air parcels.
 - CALPUFF, SCIPUFF, and SCICHEM

- Eulerian Grid Model

- Coordinate system is fixed in space.
 - CAMx and CMAQ

- Hybrid Model

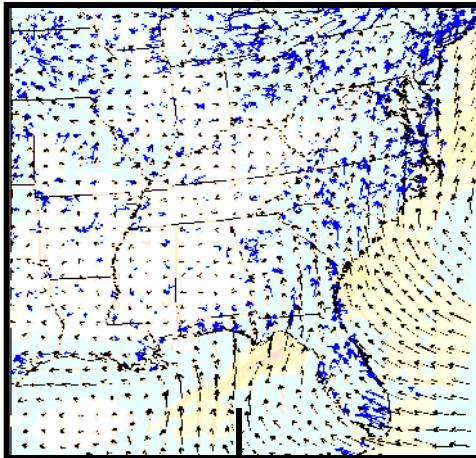
- Blending of Lagrangian parcels into Eulerian grids
 - CAMx and CMAQ with “plume-in-grid” treatments



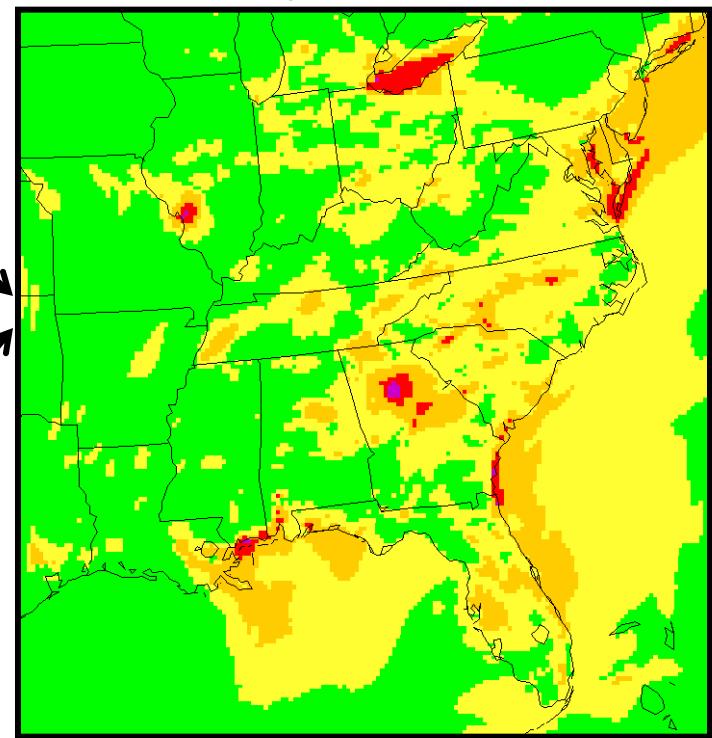


PGM MODELING SYSTEM

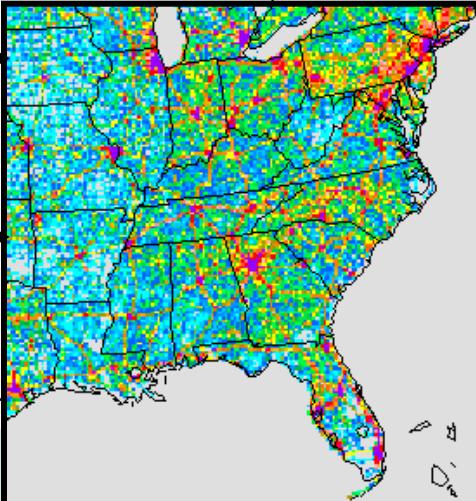
Meteorology (WRF)



Air Quality (CMAQ/CAMx)



Emissions (SMOKE)



Biogenic Emissions

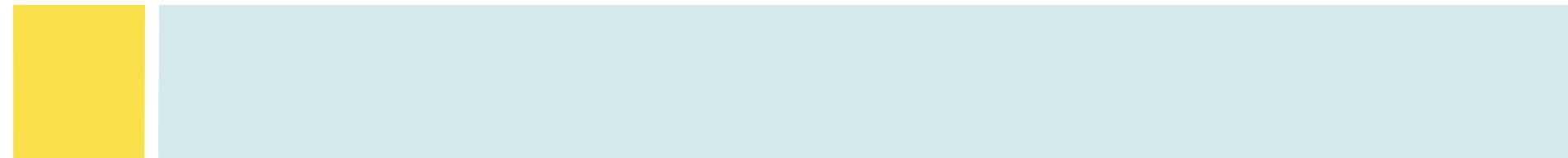
Emissions Inventory (NEI)

MOVES Rates

Hourly concentrations of criteria air pollutants and precursor pollutants



MODEL INPUTS





METEOROLOGY

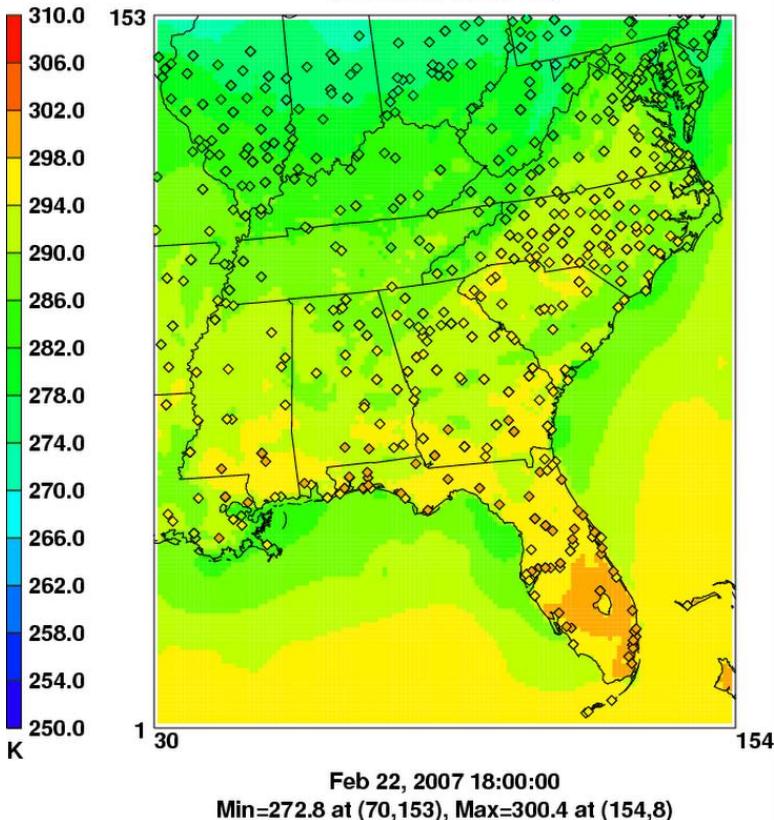
- Meteorological data for PGMs is generated using prognostic Mesoscale Meteorological Models (e.g., MM5, WRF)
 - Numerical model that solves coupled mass, energy, and momentum equations
- Modeled Meteorological Parameters
 - Air Temperature, Pressure, and Density
 - Wind Speed and Direction
 - Absolute and Relative Humidity
 - Precipitation and Cloud Parameters
 - Incoming Solar Radiation
 - Mixing Heights and Vertical Diffusivities



SURFACE PARAMETERS

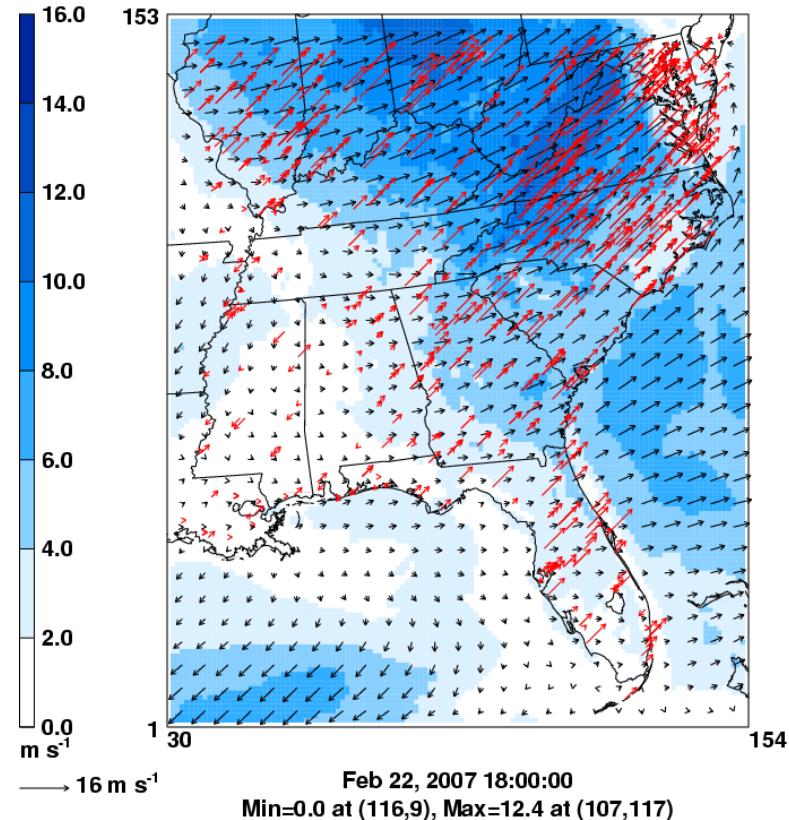
Temperature (2m)

(SESARM: 12km, 2m)



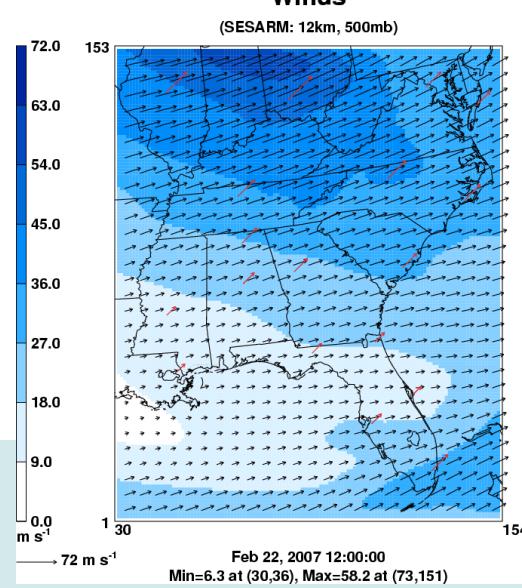
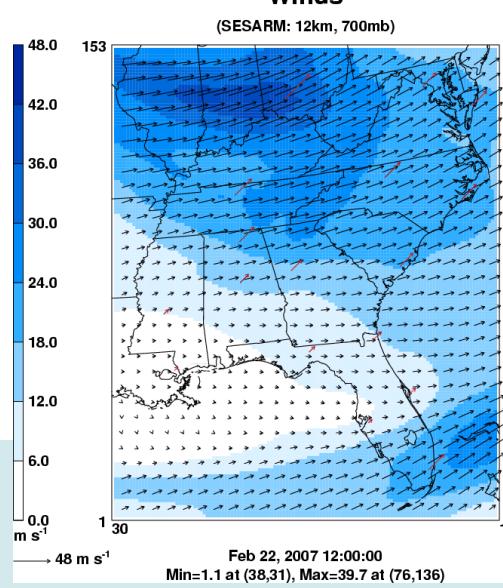
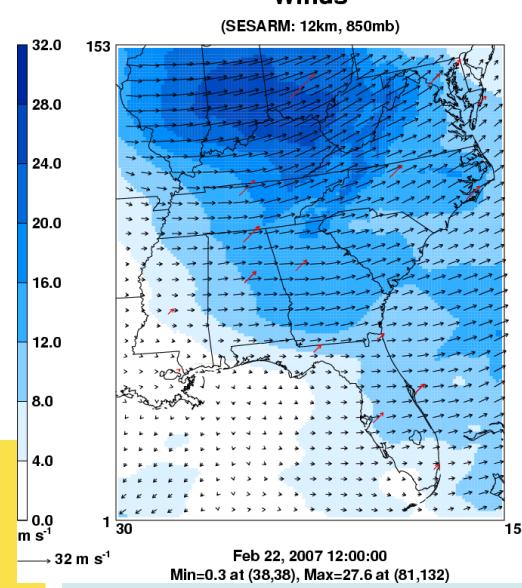
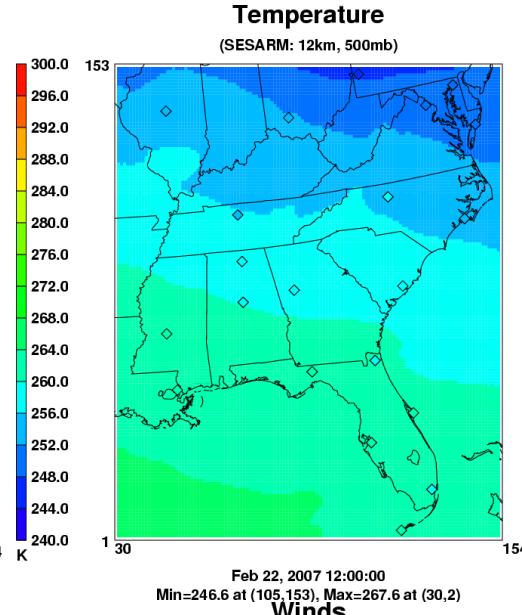
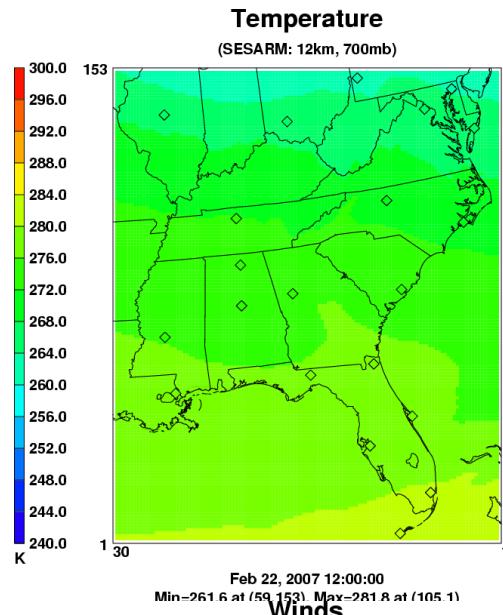
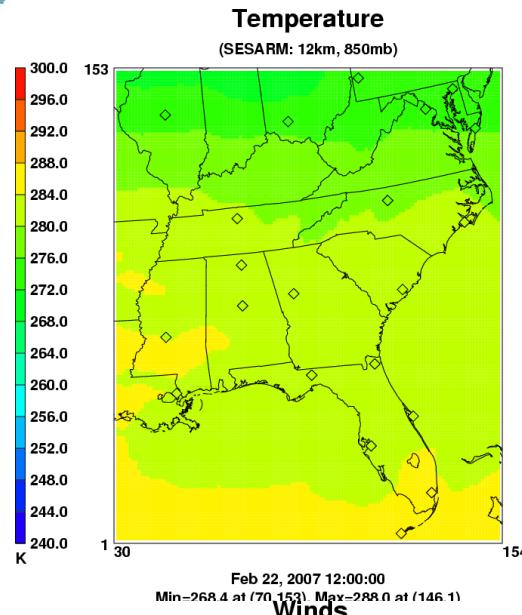
Winds

(SESARM: 12km, layer 1)





ALOFT PARAMETERS





EMISSIONS INVENTORIES

Point



Area



On-road Mobile



Non-Road Mobile



Marine



Aircraft



Rail



Fires



Biogenics





MODELED EMISSION SPECIES

CB6 Chemical Mechanism

- 90 species, 227 reactions

Gas-Phase Species

- Volatile Organic Compounds (VOCs)
 - Methane, Ethane, Propane, Ethene, Propene, 1,3-Butadiene, Isoprene, Terpenes, Benzene, Toluene, o-Xylene, Formaldehyde, etc...
- Non-VOCs
 - CO, NO, NO₂, SO₂, NH₃, HNO₃, etc...

Aerosol Phase Species

- SO₄, NO₃, NH₄, OC, EC, Soils, CM, Sea Salt

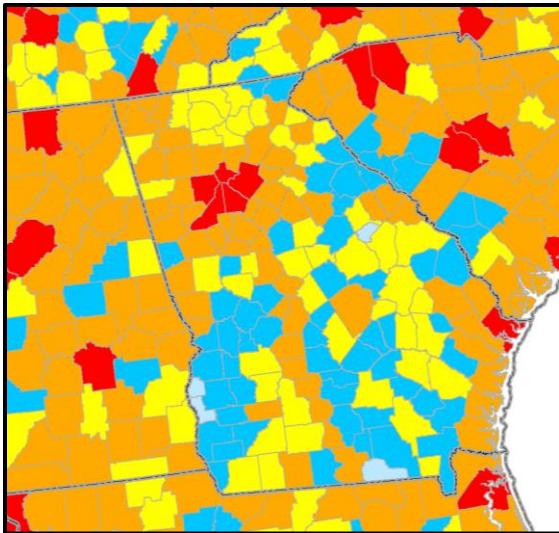


SMOKE MODELING

- Sparse Matrix Operator Kernel Emissions (SMOKE)
- Temporal Allocation
 - Annual → monthly → weekly → daily → hourly
- Spatial Allocation
 - County level → grid cell level (e.g., 12-km)
 - Spatial surrogates (population, VMT, etc)
- Pollutant Speciation
 - NOx → NO₂ and NO
 - VOCs → Methane, Ethane, Propane, Ethene, Propene, 1,3-Butadiene, Isoprene, Terpenes, Benzene, Toluene, o-Xylene, Formaldehyde, etc...
 - PM_{2.5} → Sulfate, Nitrate, Organic Carbon, Elemental Carbon, etc...

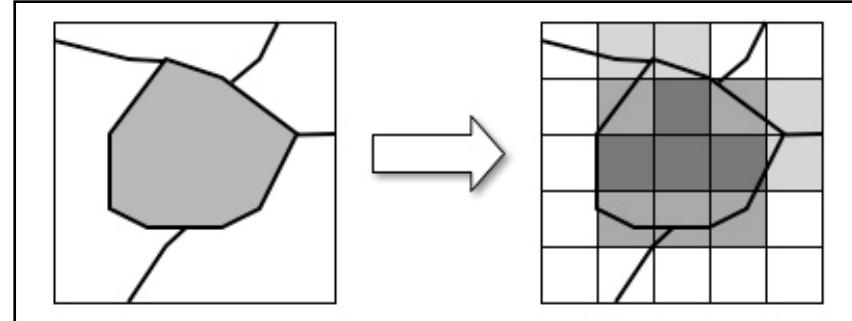


EMISSIONS MODELING

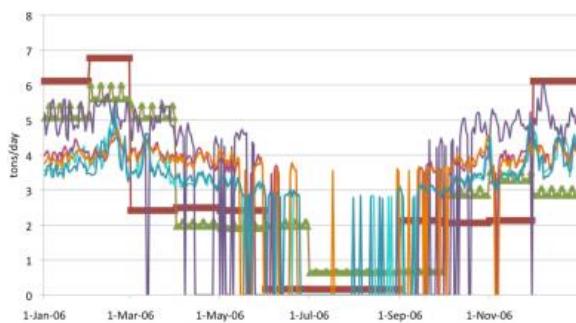


Annual NOx emissions

+



+

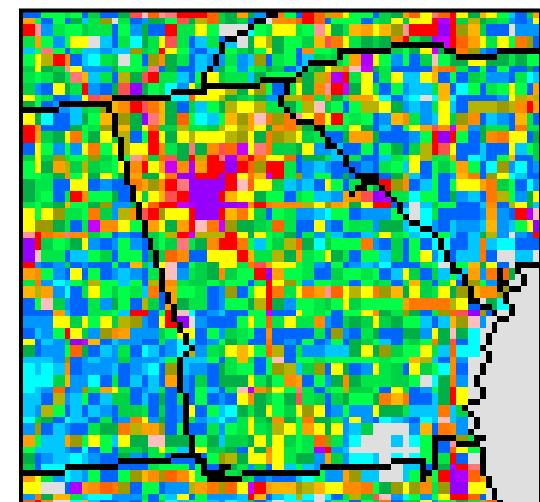


Annual → Hourly

+

**NO
VS.
NO₂**

→



Hourly NO emissions



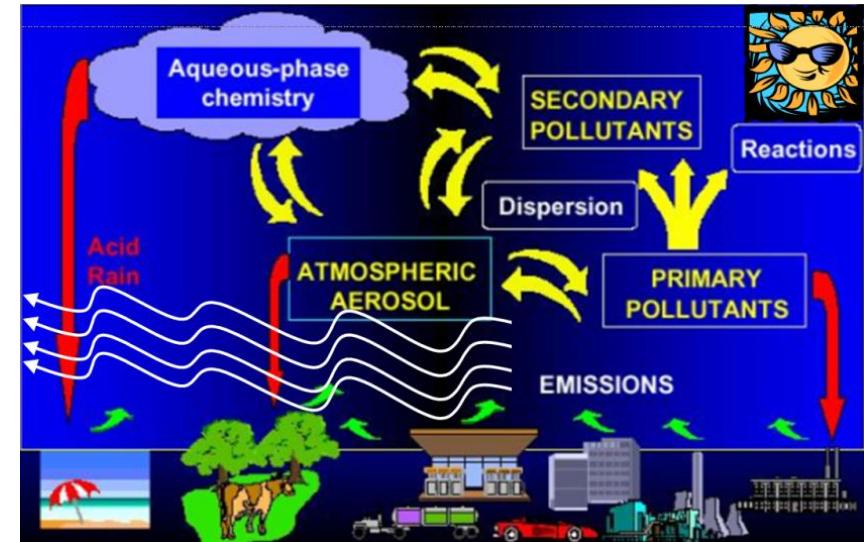
HOW PGMS WORK





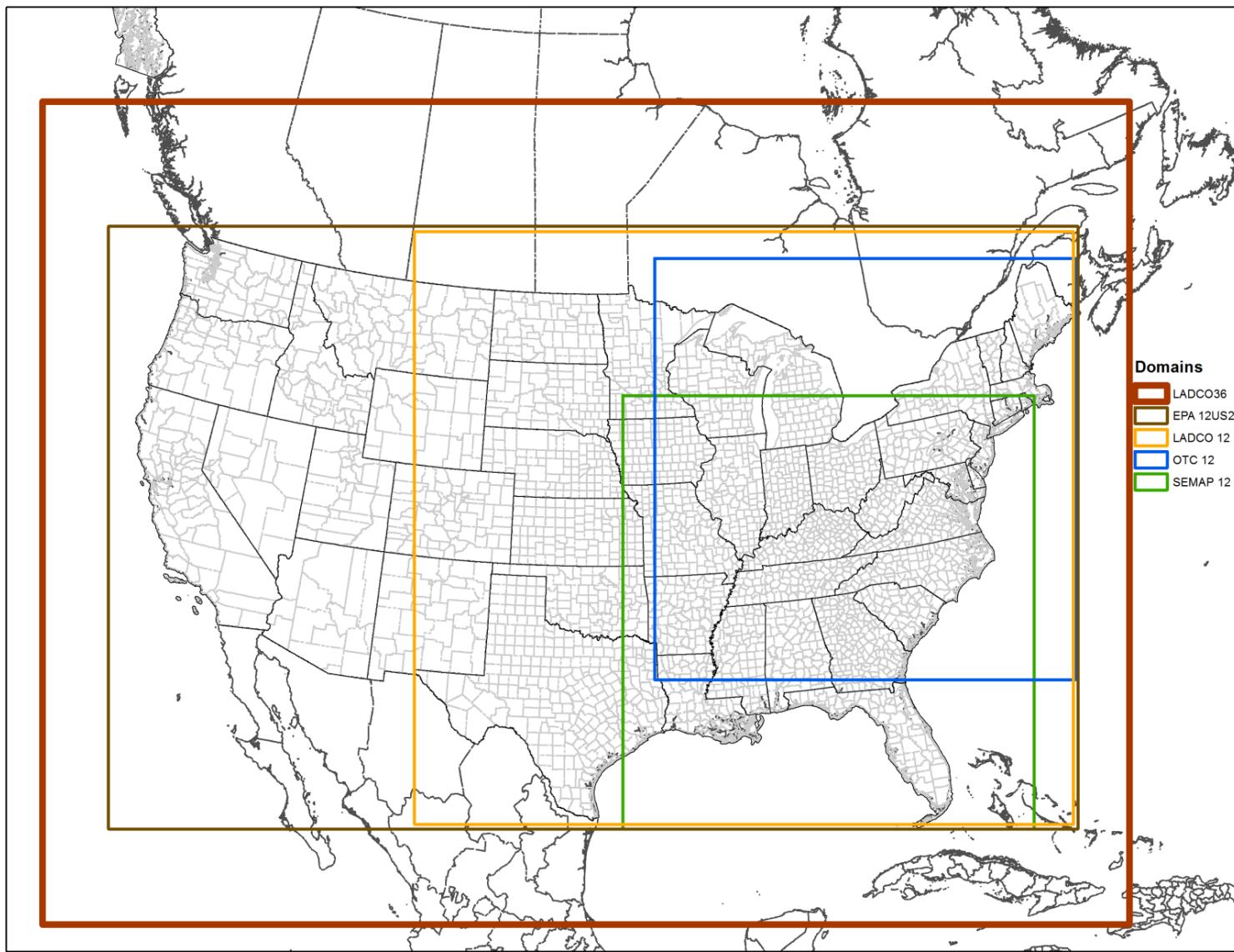
PGM MODEL PROCESSES

- Emissions (source)
- Transport
 - Advection (transport by mean/resolved wind)
 - Turbulent diffusion (transport by unresolved motion)
- Chemical transformations (source and sink)
 - Gas-phase chemistry
 - Aerosol dynamics
 - Heterogeneous chemistry
- Deposition (sink)
 - Wet deposition
 - Dry deposition





EXAMPLE MODELING DOMAINS





INSTANTLY MIXED GRID CELLS

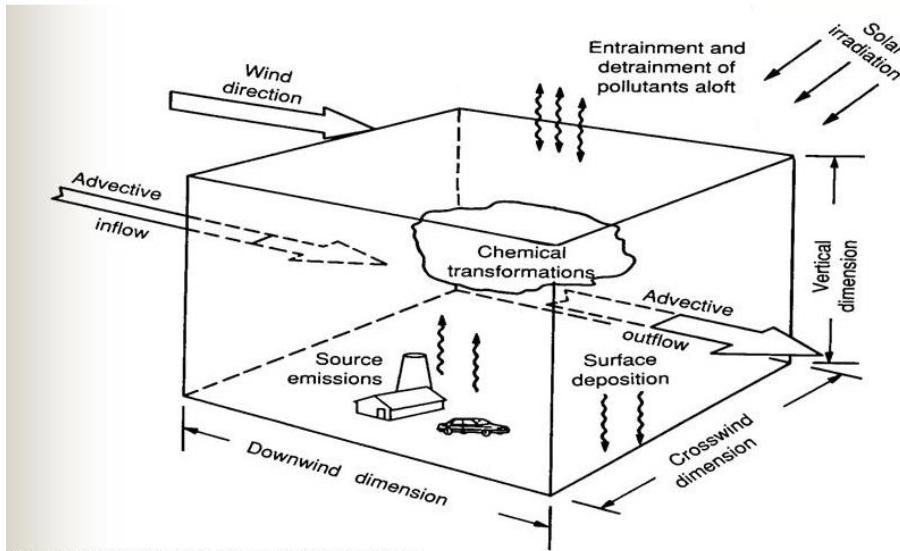
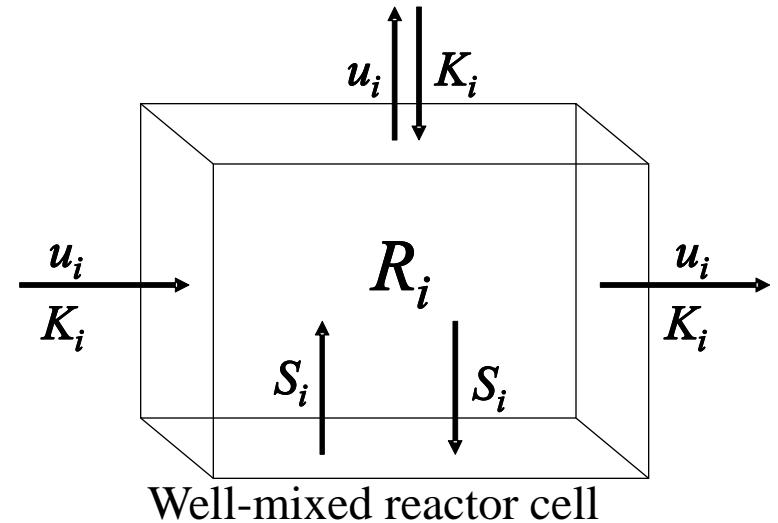
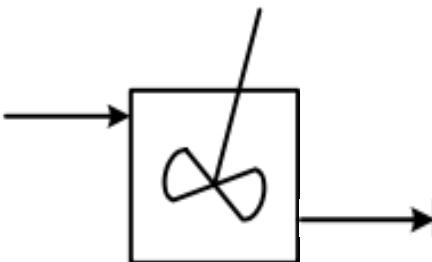


Figure from <http://irina.colorado.edu/lectures/Lec29.htm>



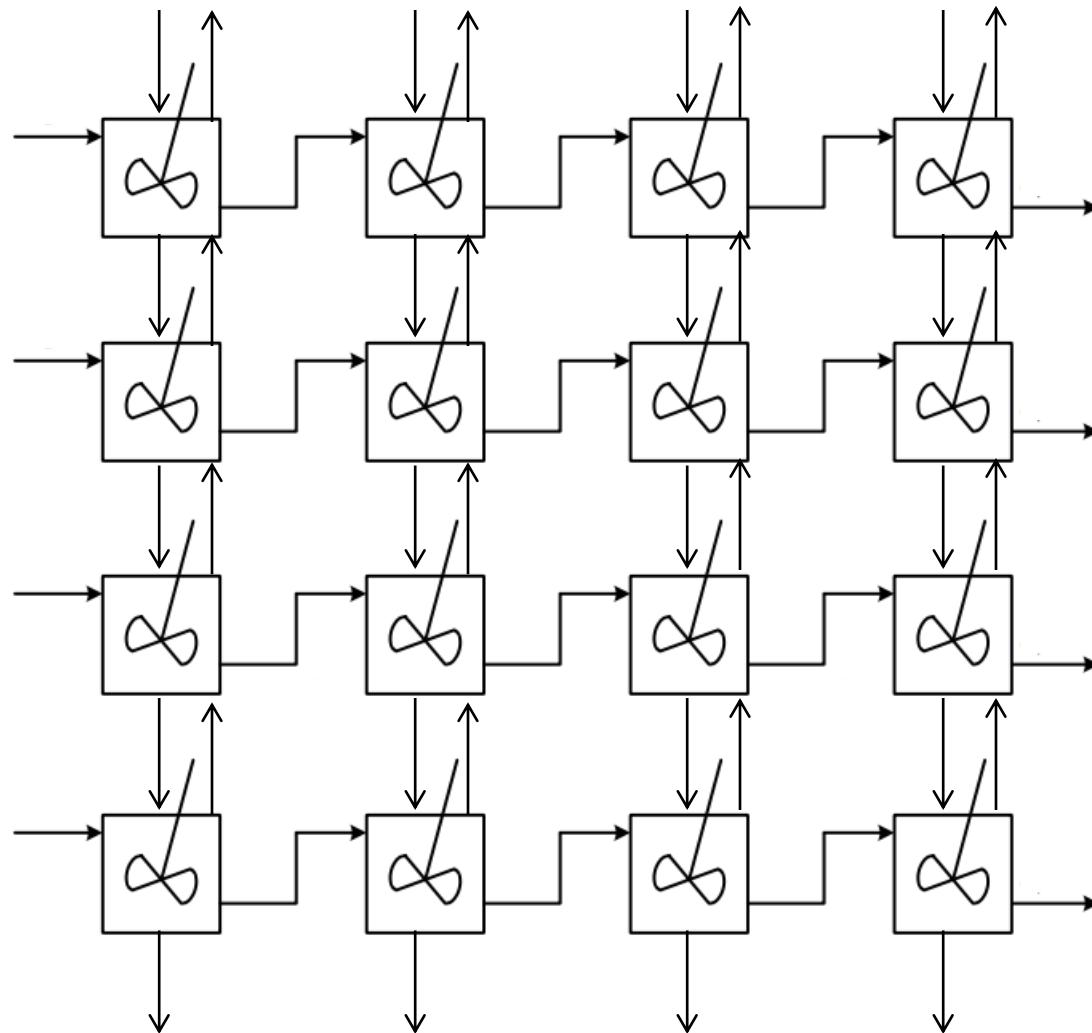
Well-mixed reactor cell



$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{u} c_i) = \nabla \cdot (\mathbf{K} \nabla c_i) + R_i + S_i$$

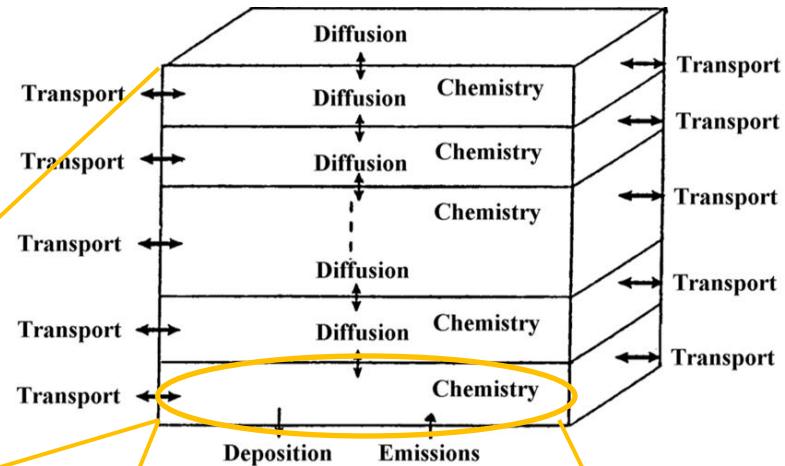
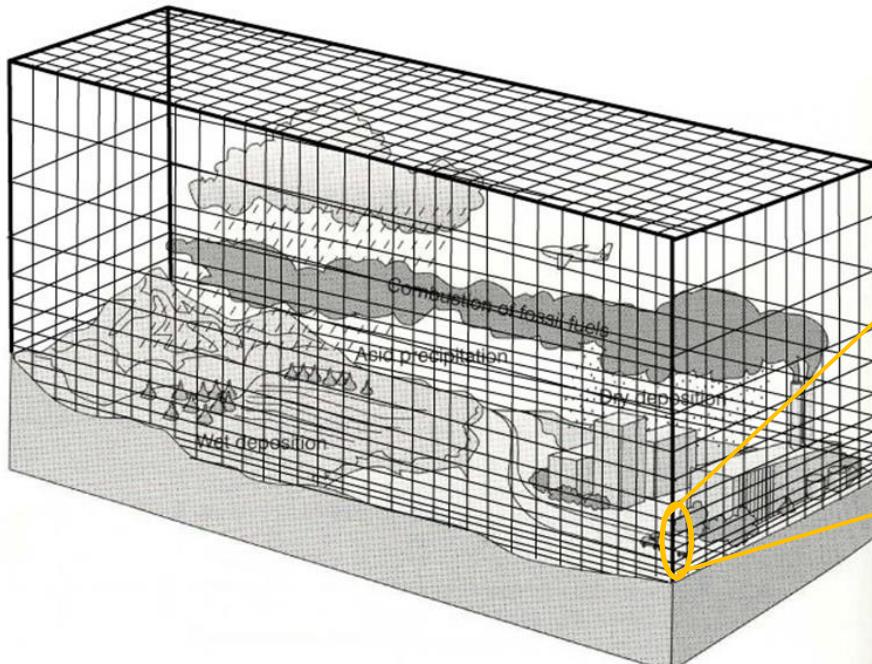


SERIES OF MIXED REACTORS



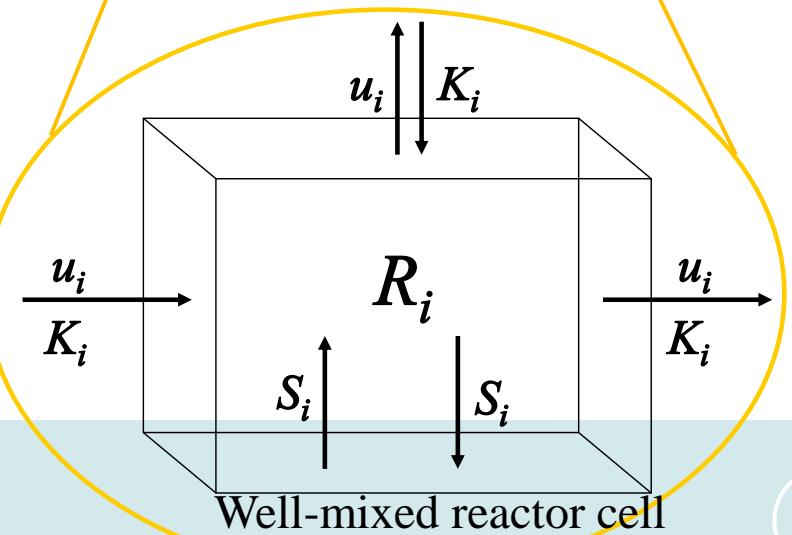


PHOTOCHEMICAL GRID MODELS



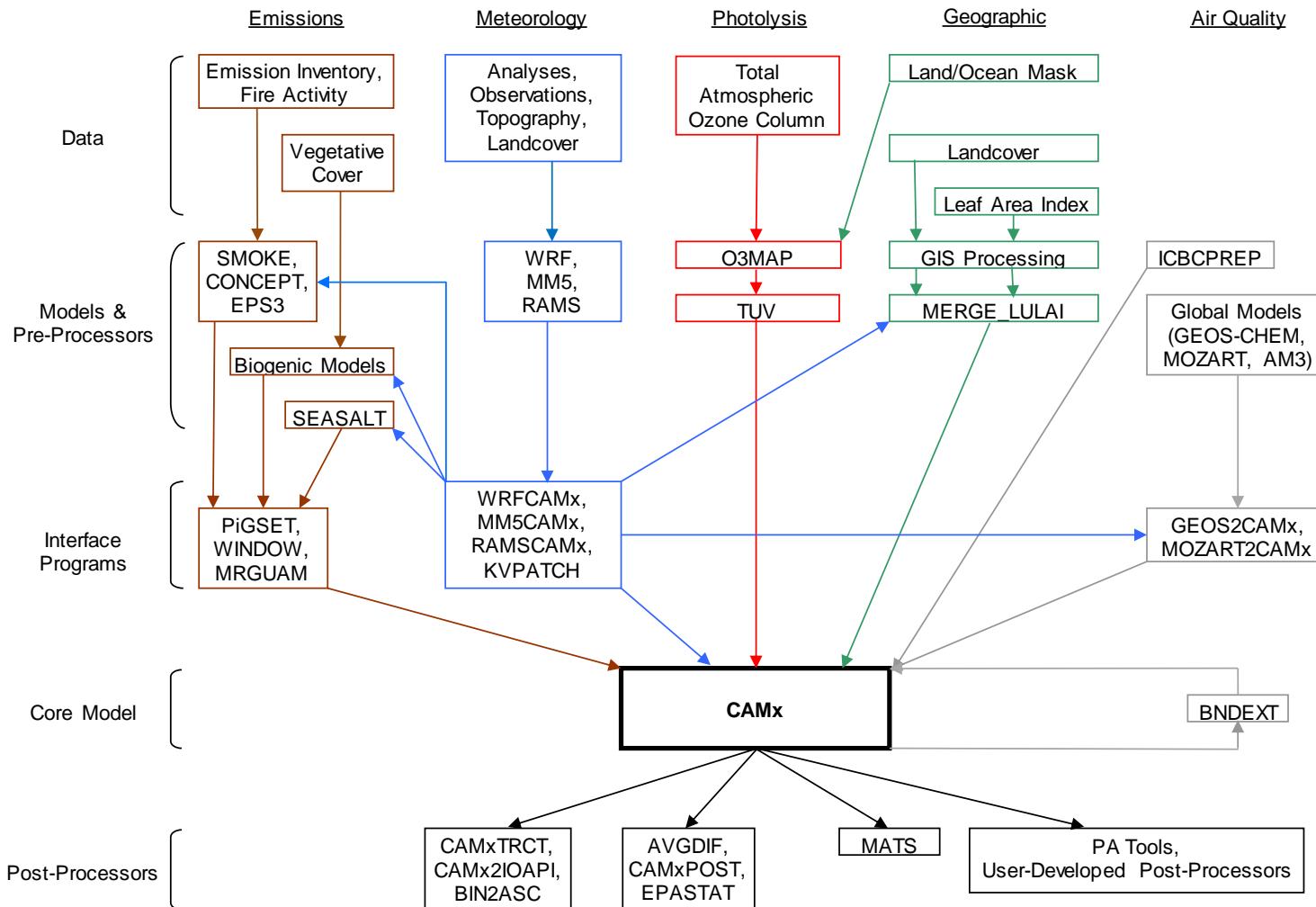
Atmospheric Diffusion Equation

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{u} c_i) = \nabla \cdot (\mathbf{K} \nabla c_i) + R_i + S_i$$





CAMx MODELING SYSTEM



File Formatting

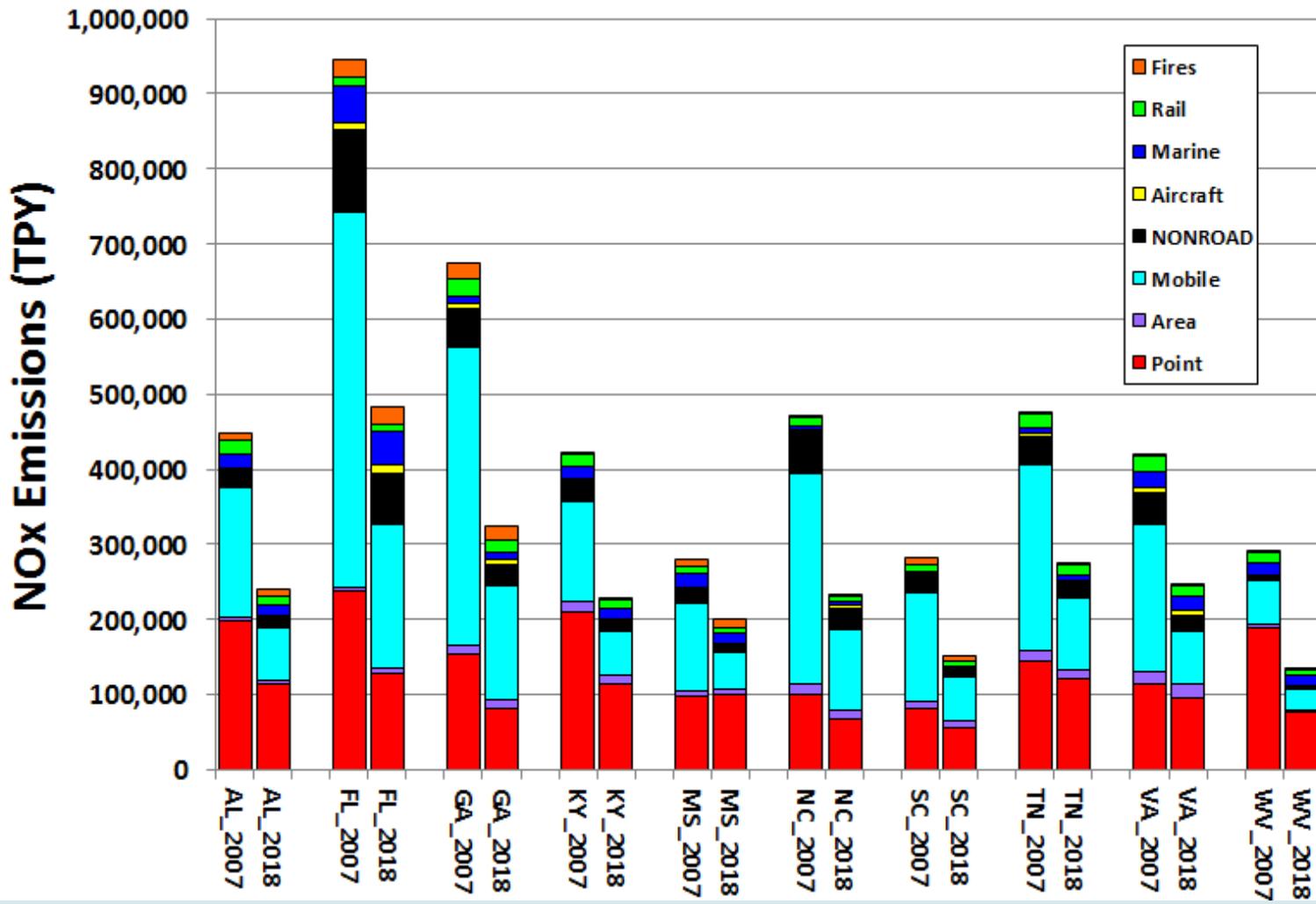
Performance

Regulatory

Probing Tools



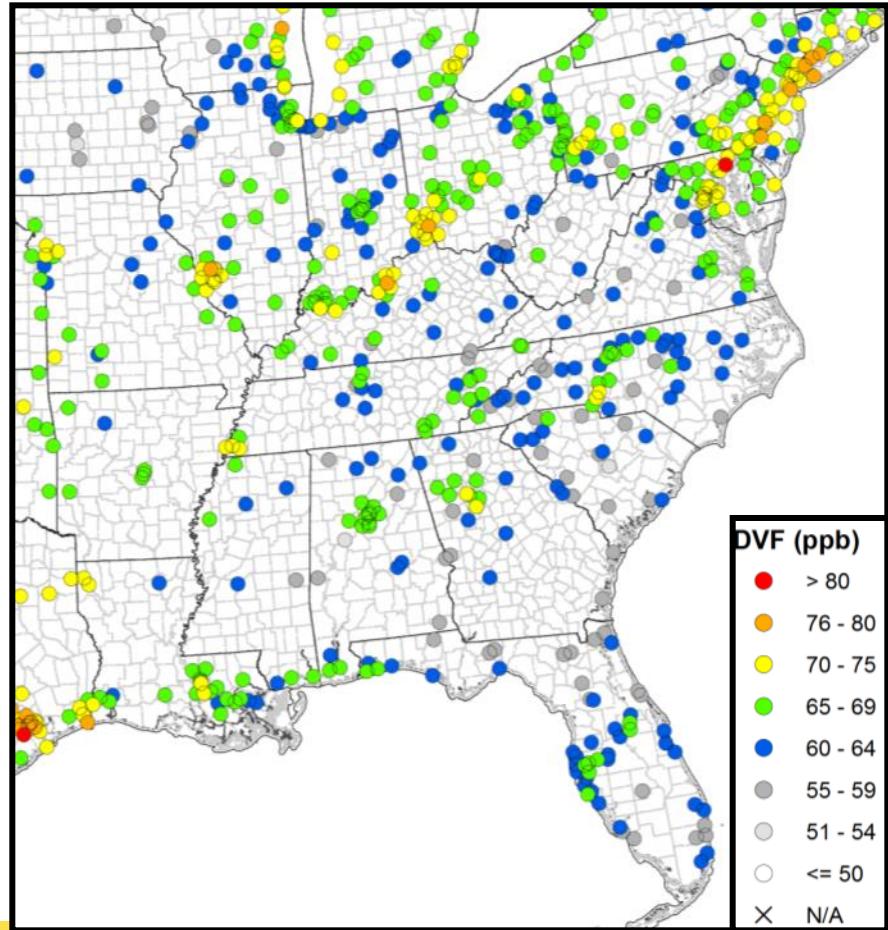
NO_x EMISSION PROJECTIONS



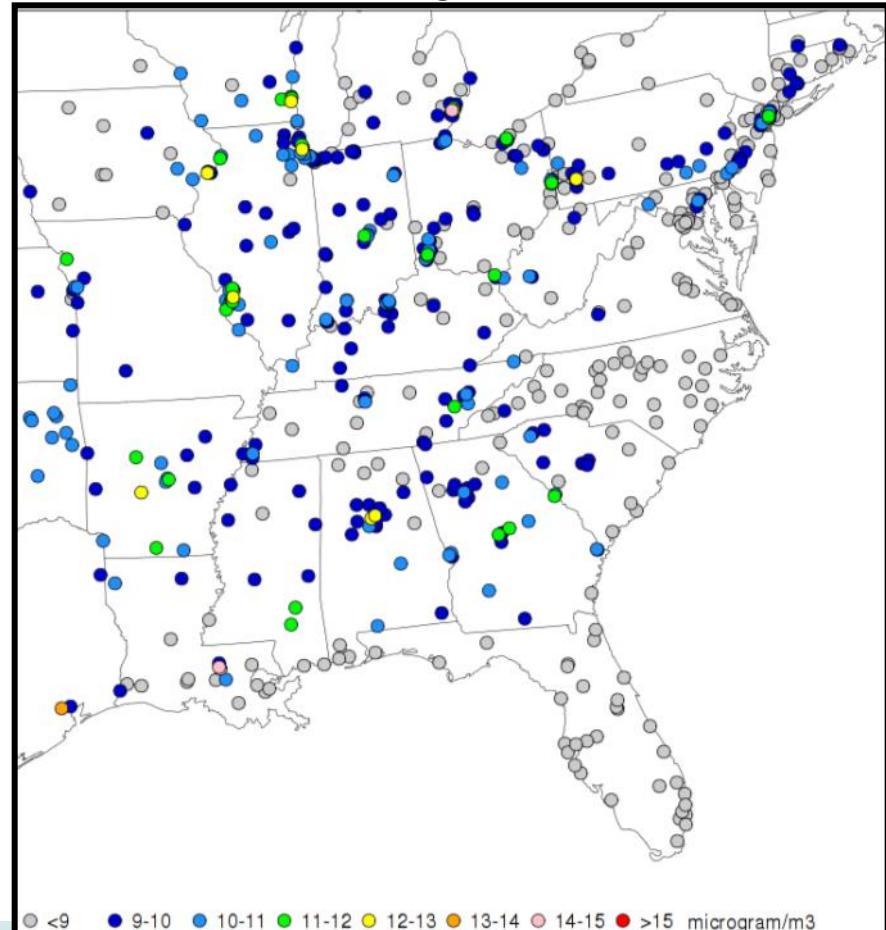


2018 PROJECTIONS

2018 Ozone Projections

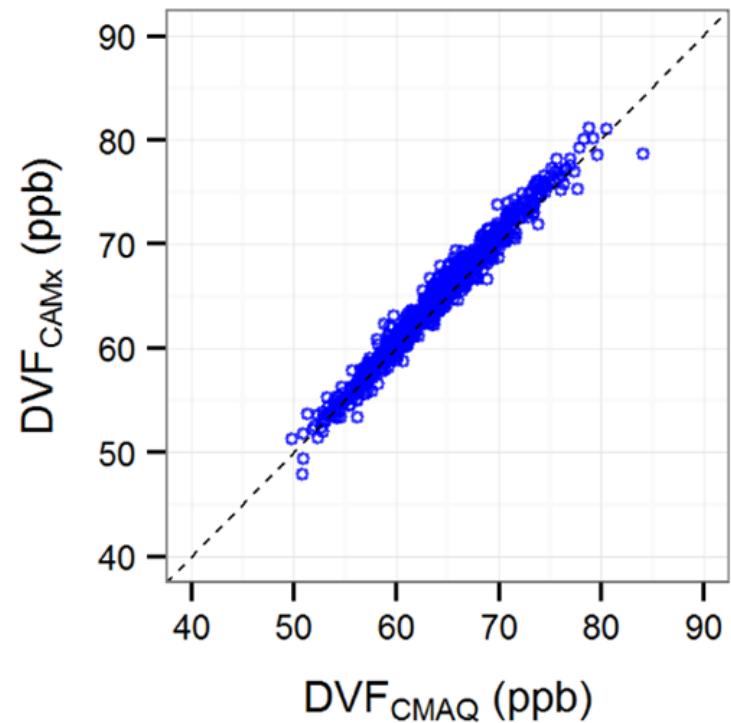
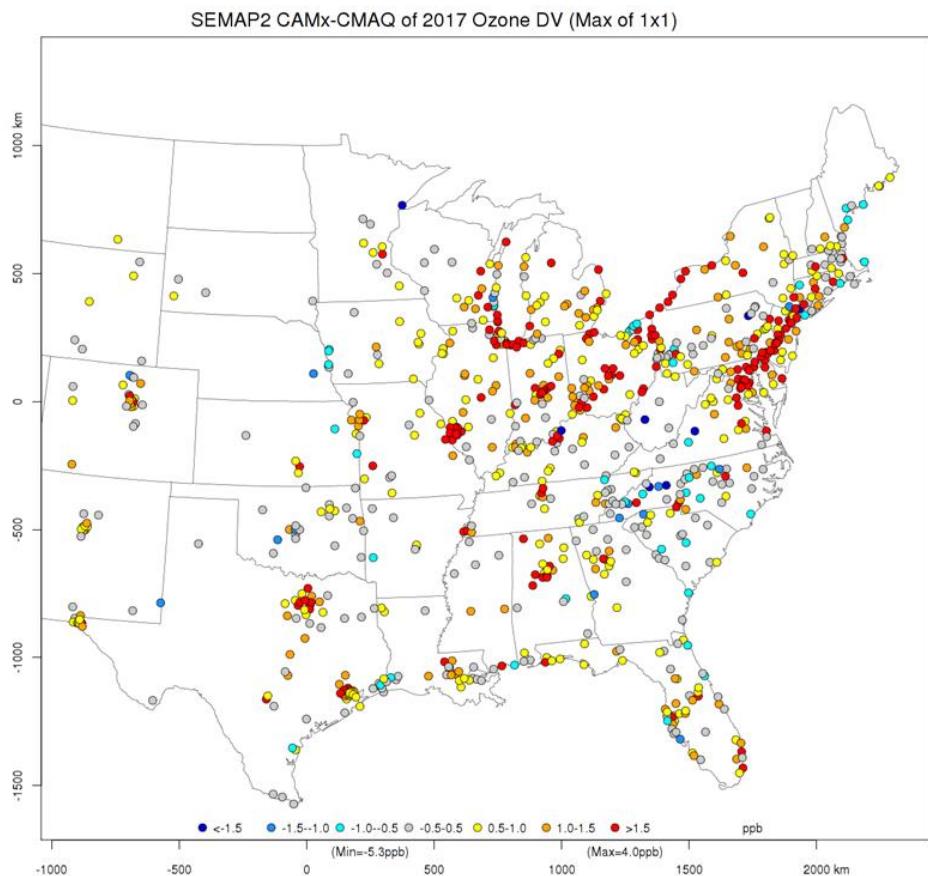


2018 PM_{2.5} Projections





CAMx vs. CMAQ

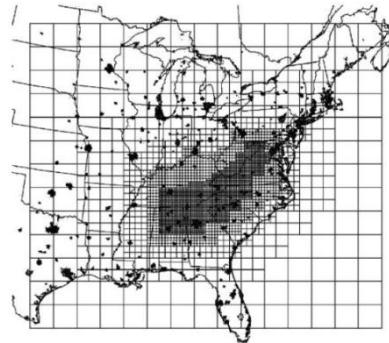




EVOLUTION OF PGMS

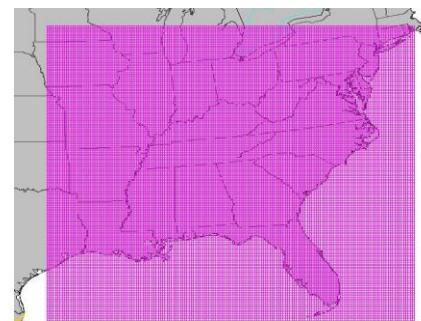
- **CIT → URM → URM-1ATM**

- CIT = California/Carnegie Institute of Technology Model
- URM = Urban-to-Regional Multiscale Model
- URM-1ATM = Urban-to-Regional Multiscale - One Atmosphere Model (Boylan, 2002)



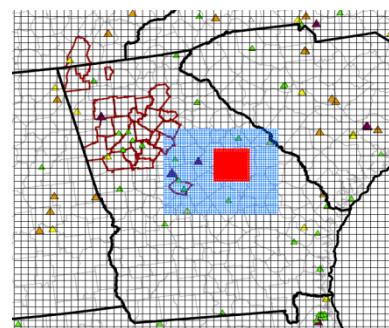
- **MAQSIP → CMAQ**

- MAQSIP = Multiscale Air Quality Simulation Platform
- CMAQ = Community Multiscale Air Quality Model



- **UAM → UAM-V → CAMx**

- UAM = Urban Airshed Model
- UAM-V = Variable-Grid Urban Airshed Model
- CAMx = Comprehensive Air Quality Model with Extensions





MODEL PERFORMANCE EVALUATION



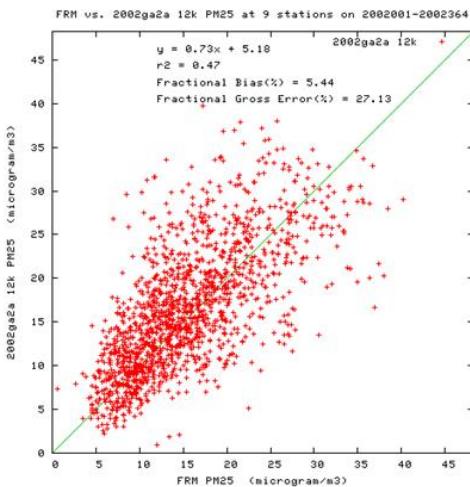


**“All models are wrong.
Some are useful.”**

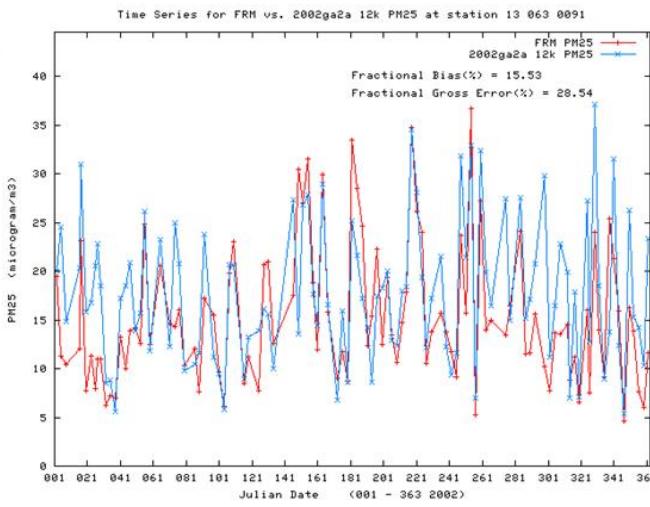




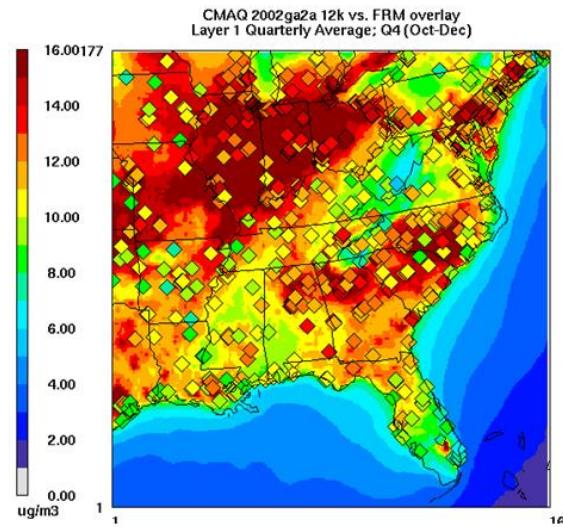
COMMON MPE PLOTS



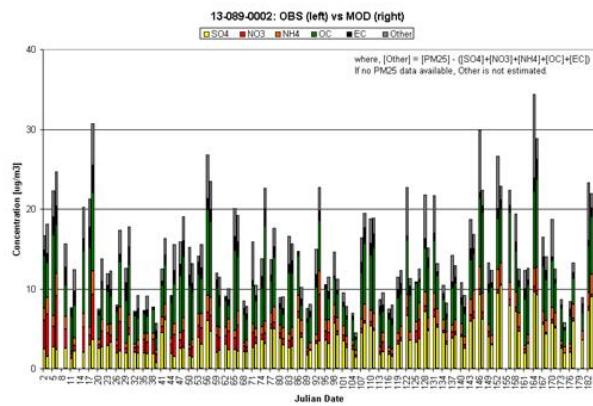
(a)



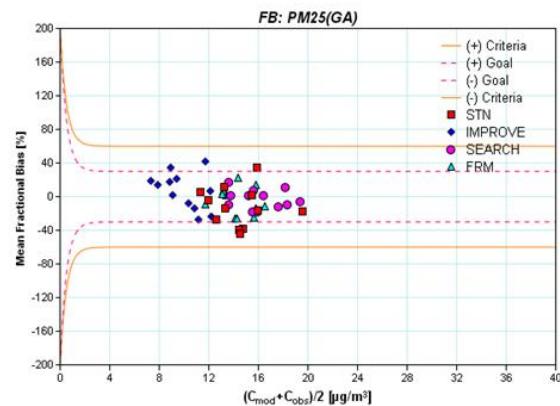
(b)



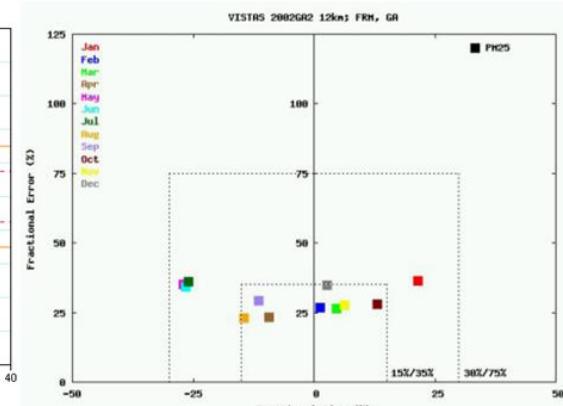
(c)



(d)



(e)

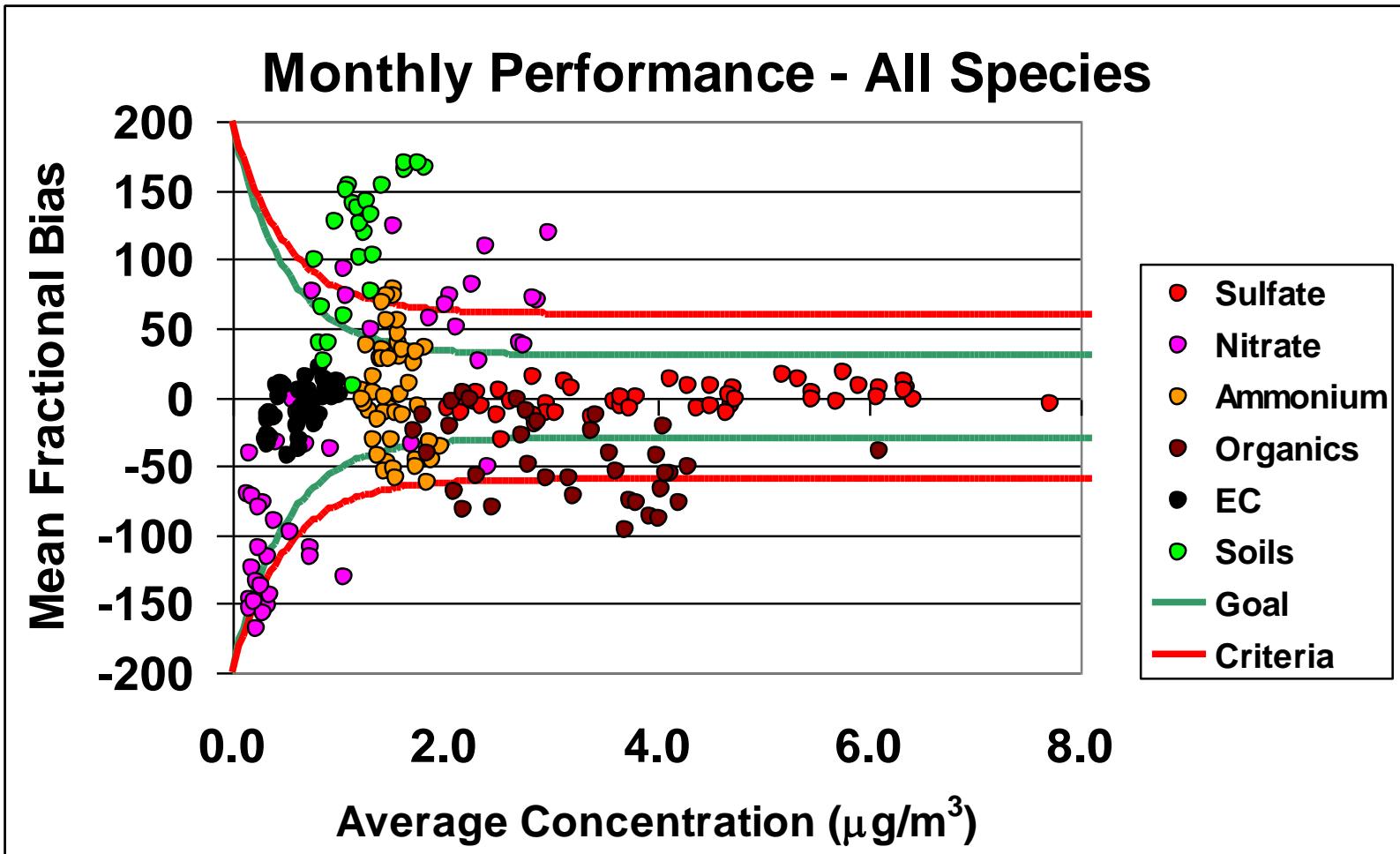


(f)

Russell A., Boylan J., Napelenok S. (2012) Air Pollution Data for Model Evaluation and Application. *EM*, May 2012, pp. 30-35.



PM_{2.5} MODEL PERFORMANCE



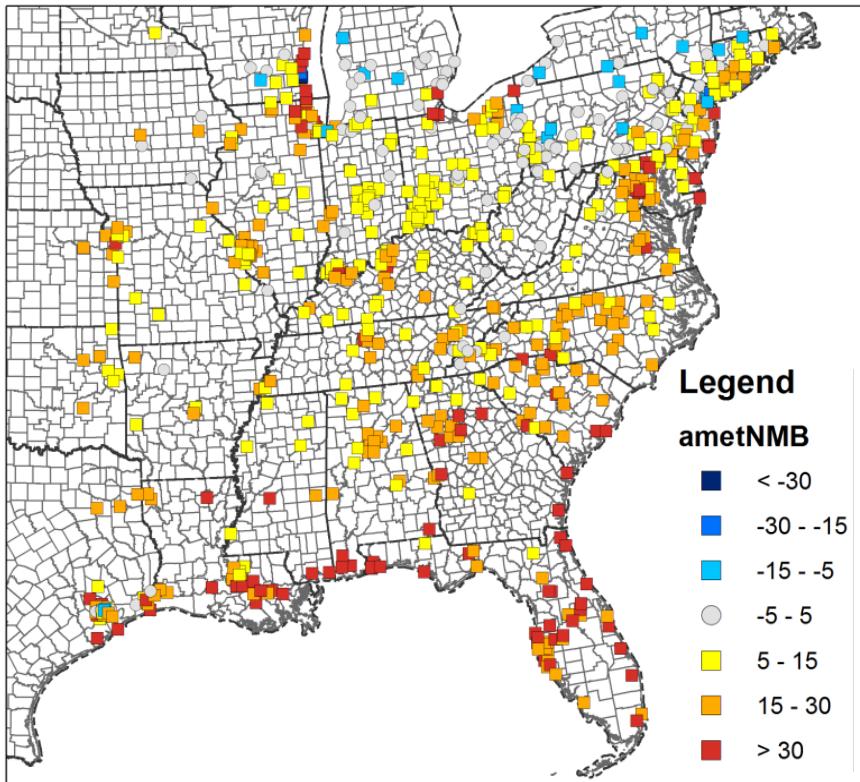
Boylan, J.W. and Russell, A.G. (2006). PM and Light Extinction Model Performance Metrics, Goals, and Criteria for Three-Dimensional Air Quality Models; *Atmos. Environ.*, Volume 40, pp. 4946-4959.

Emery, C., Liu, Z., Russell, A. G., Odman, M. T., Yarwood, G., & Kumar, N. (2017). Recommendations on Statistics and Benchmarks to Assess Photochemical Model Performance. *Journal of the Air & Waste Management Association*, 67(5), 582-598. doi:10.1080/10962247.2016.1265027.

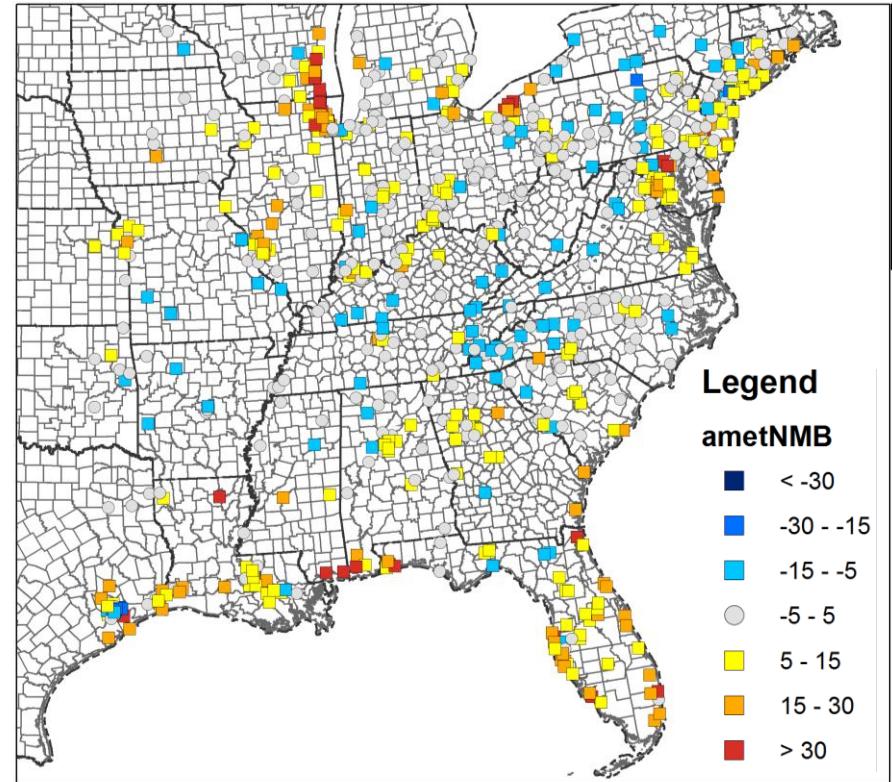


8-HOUR OZONE NMB - AUGUST

BEFORE

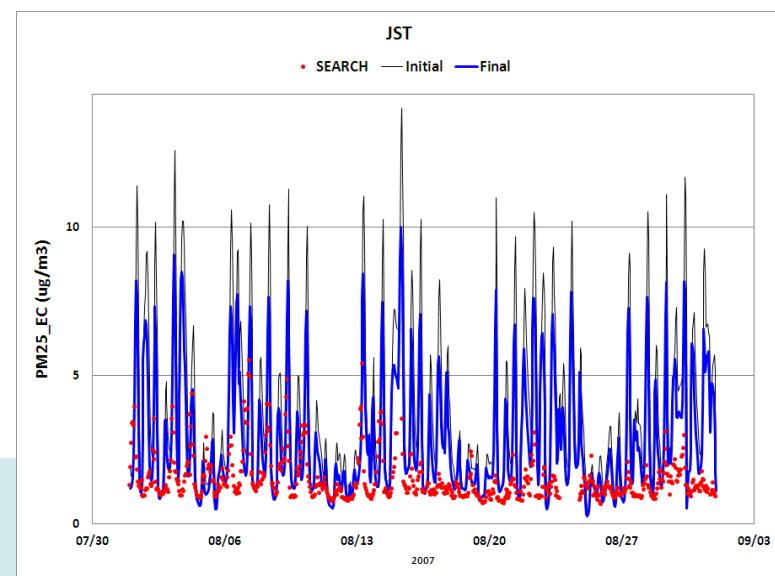
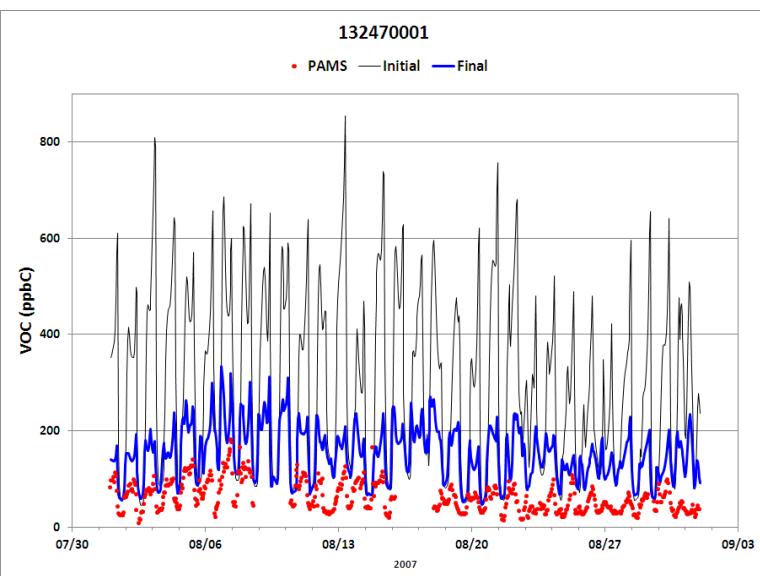
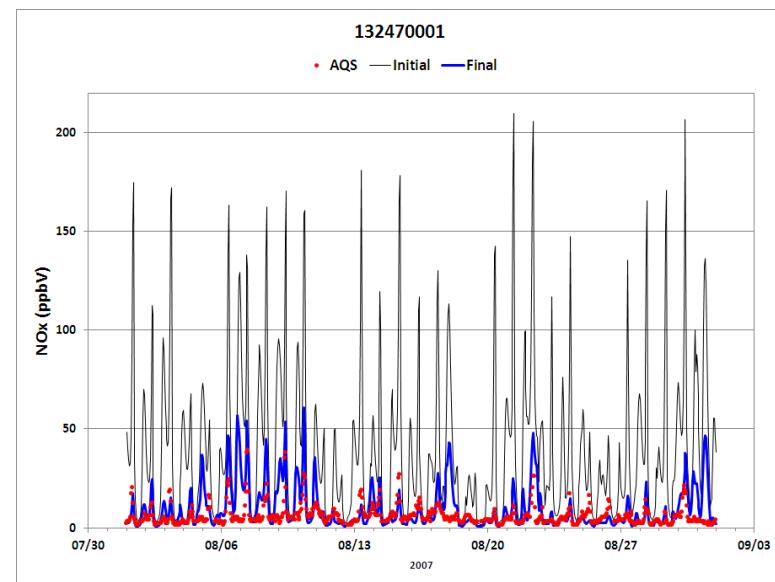
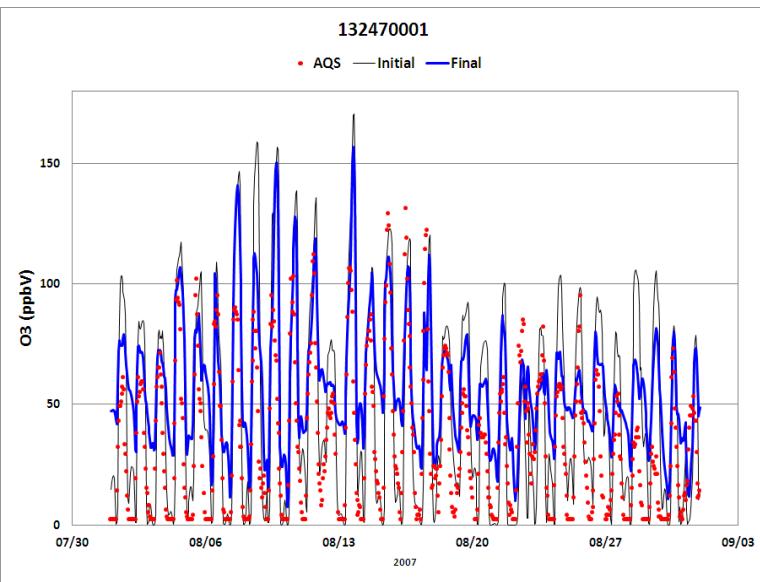


AFTER





TIME SERIES PLOTS - AUGUST





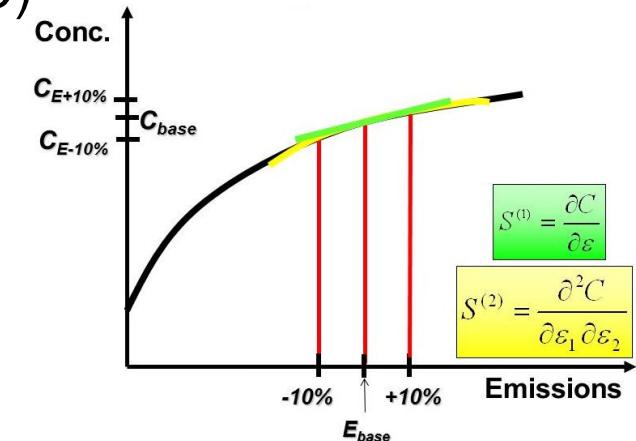
PROBING TOOLS





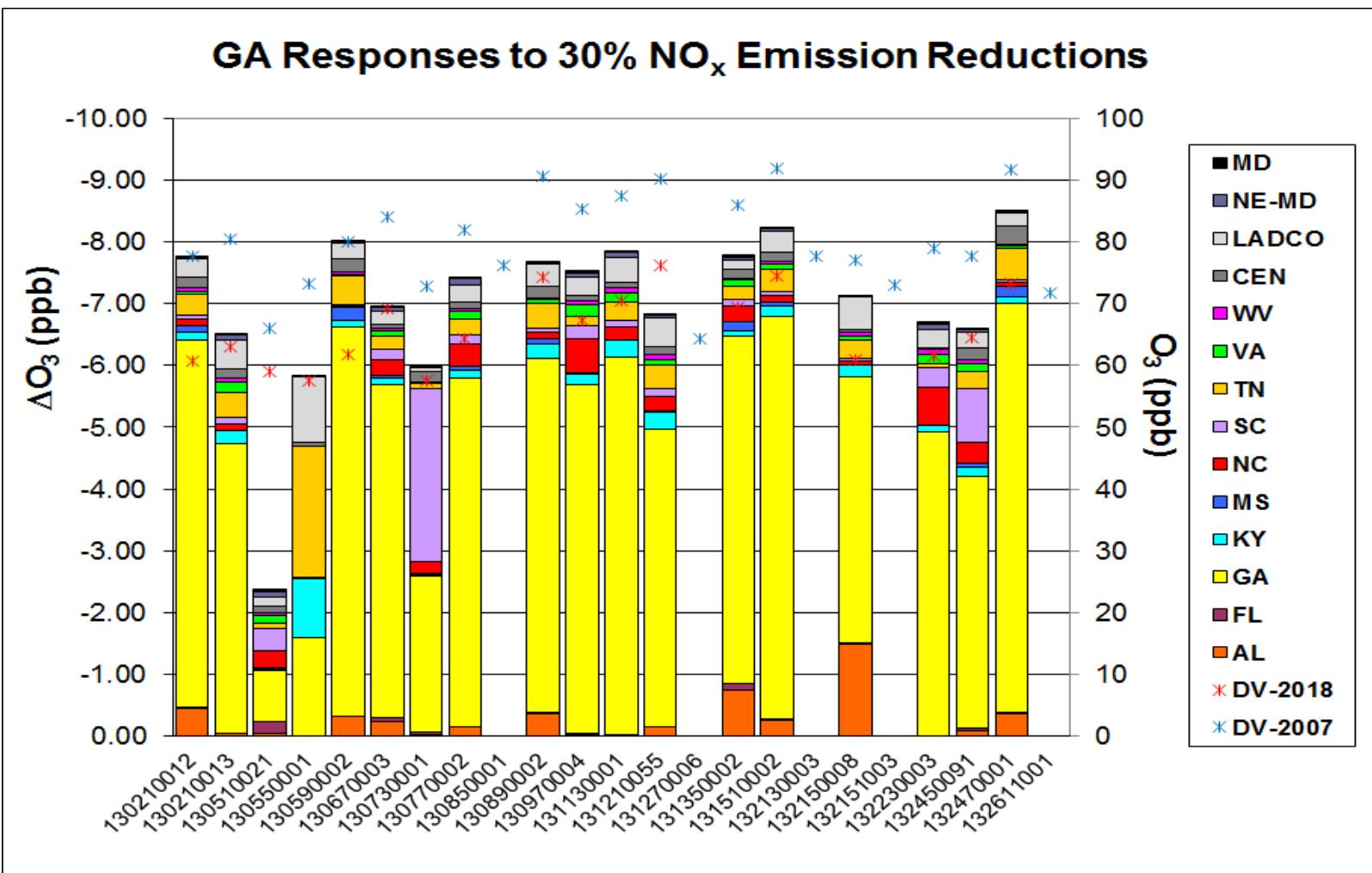
COMMON PROBING TOOLS

- Sensitivity vs. Source Apportionment
- Brute Force Sensitivity
 - $\pm 10\%$, $\pm 30\%$, $\pm 50\%$, $\pm 100\%$
- Source Apportionment Tagging
 - CAMx \rightarrow PSAT ($PM_{2.5}$), OSAT/APCA (ozone)
 - CMAQ \rightarrow ISAM ($PM_{2.5}$ and ozone)
- Decoupled Direct Method
 - First order (DDM)
 - Higher Order (HDDM)
 - Ozone and $PM_{2.5}$



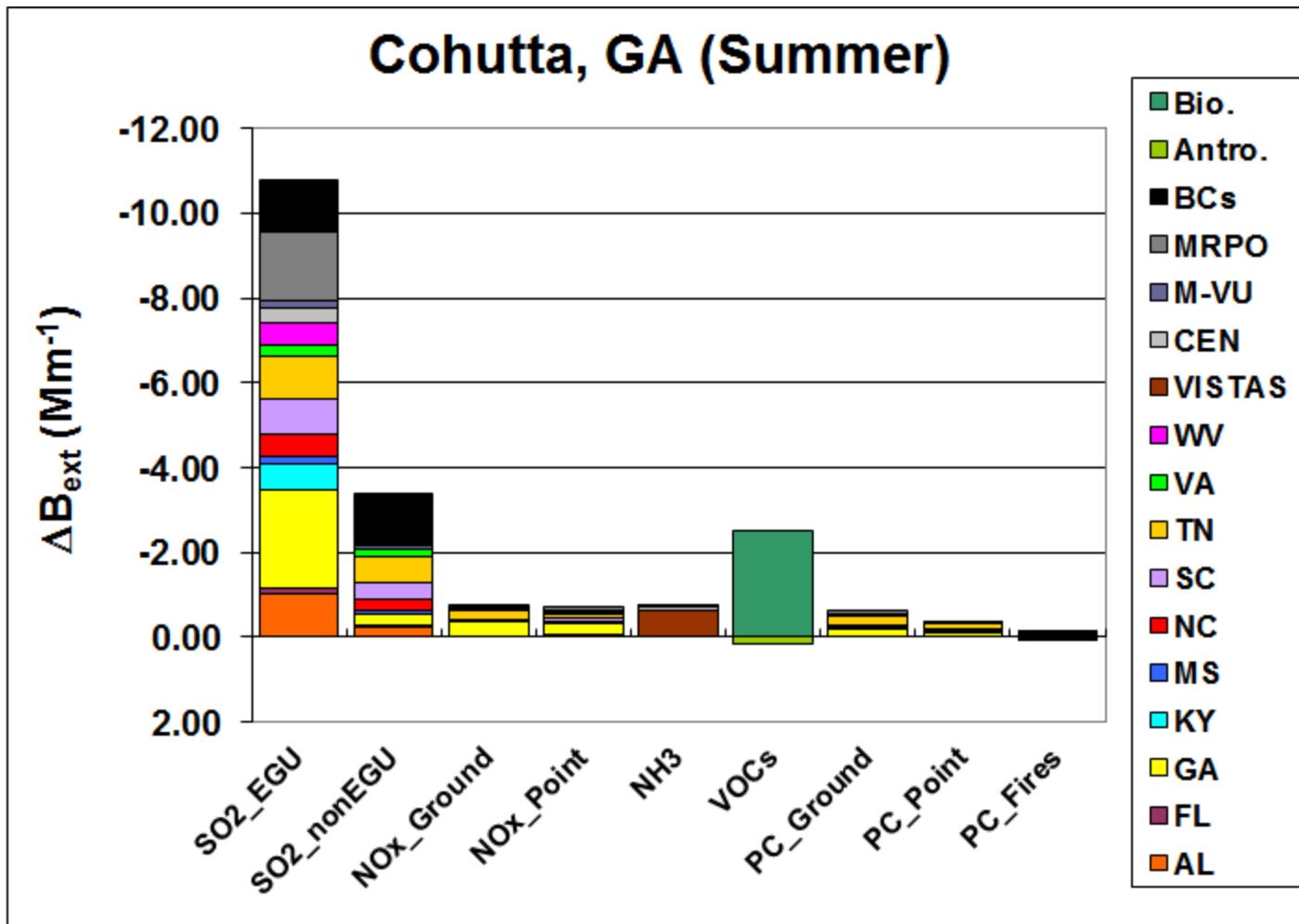


2018 EMISSION SENSITIVITIES





EMISSION SENSITIVITIES





SEMAP CMAQ BRUTE FORCE SENSITIVITIES

Monitor ID	State	County	2017 Projected Average Design Value	2017 Projected Maximum Design Value	AL	FL	GA	KY	MS	NC	SC	TN	VA	WV
90013007	Connecticut	Fairfield	79.2	81.5	0.07	0.01	0.09	0.53	0.05	0.22	0.05	0.12	1.11	0.59
211850004	Kentucky	Oldham	78.8	81.2	0.16	0.02	0.03	20.97	0.06	0.06	0.04	0.74	0.02	0.09
240251001	Maryland	Harford	78.3	80.9	0.28	0.08	0.27	0.93	0.03	0.09	0.05	0.21	5.06	1.81
361030002	New York	Suffolk	77.8	77.8	0.10	0.02	0.11	0.27	0.03	0.17	0.04	0.16	0.84	0.47
420031008	Pennsylvania	Allegheny	77.3	81.7	0.03	0.02	0.03	0.87	0.02	0.02	0.02	0.27	0.02	0.98
90019003	Connecticut	Fairfield	75.1	77.9	0.07	0.01	0.09	0.51	0.03	0.24	0.05	0.15	1.20	0.60
340071001	New Jersey	Camden	74.3	76.5	0.07	0.03	0.05	0.33	0.07	0.02	0.02	0.05	0.08	0.76
390610006	Ohio	Hamilton	74.1	78.0	0.64	0.05	0.73	8.62	0.20	0.10	0.08	0.85	0.08	0.89
420030008	Pennsylvania	Allegheny	73.9	76.9	0.01	0.01	0.00	0.12	0.04	-0.01	0.00	0.06	0.00	0.86
421010024	Pennsylvania	Philadelphia	73.9	76.1	0.40	0.07	0.36	1.07	0.06	0.08	0.07	0.38	1.09	1.98

Nonattainment

Maintenance

Significant impact

Self impact



COMPUTER RESOURCES





HARDWARE OPTIONS

System	CPUs	Type	RAM	Storage	Cost
Leased Server	72	1 TB	12 TB (RAID5)	24 TB	\$3,379/month + \$17,500/month
Standalone Workstation	36	1 TB	22 TB (RAID6)	40 TB	\$40,000 (upfront) + \$8,300 (upfront)
Cloud Computing	64	1 TB	2 TB	40 TB	\$5,000/month + \$1,600/month



WHY SO MUCH COMPUTER POWER?

- Need to solve the Atmospheric Diffusion Equation for each species in each grid cell for each time step
- $(269 * 242 \text{ horizontal grid cells}) \times (25 \text{ vertical layers}) \times (100 \text{ species}) \times (4 \text{ time step/hour}) \times (24 \text{ hours/day}) \times (365 \text{ days/year})$
- **IN AN ANNUAL SIMULATION, NEED TO SOLVE OVER $5,700,000,000,000$ PARTIAL DIFFERENTIAL EQUATIONS!!!!**

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{u} c_i) = \nabla \cdot (\mathbf{K} \nabla c_i) + R_i + S_i$$



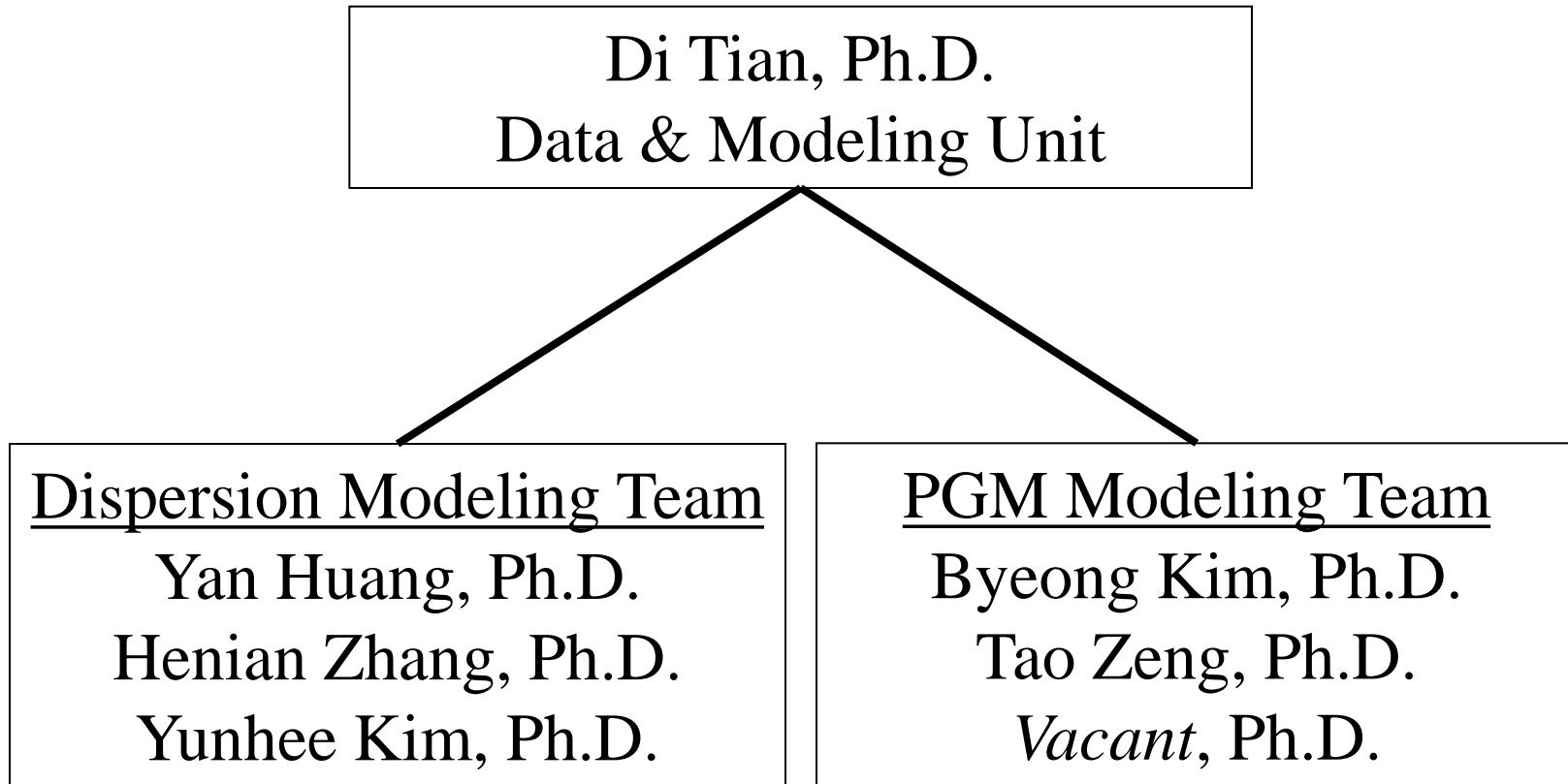


PERSONNEL





DMU ORGANIZATIONAL STRUCTURE





MODELING STAFF QUALIFICATIONS

- Advanced degree in chemical engineering, mechanical engineering, environmental engineering, atmospheric sciences, or meteorology
- Experience running numerical models
- Knowledge of EPA rules and guidance related to modeling
- Background in scientific computer programming (FORTRAN), database management (MYSQL and ACCESS), Geographic Information System (GIS), and experience with Linux or Unix.



MODELING STAFF RESPONSIBILITIES

- Run the Model (this is the EASY part)
- Develop Modeling Objectives
- Design Modeling Approach
- Create Model Inputs
- Post-Process Model Outputs
- Analyze and Interpret Results
- Identify Errors and Debug Code
- Document Results

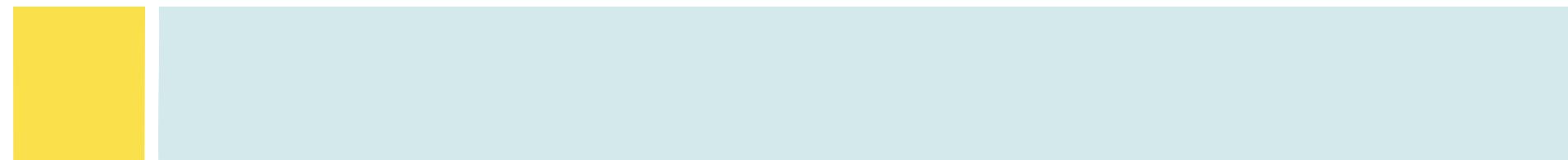


ON-GOING STAFF DEVELOPMENT

- **Formal Training**
 - WRF, SMOKE, CMAQ, CAMx, BenMAP, CMAS MPE
- **Attend National Conferences**
 - CMAS, AWMA, EPA Workshops, others...
- **Participate on National Workgroups Calls**
 - EPA, AAPCA, NACAA
- **Read Journal Articles**
- **Read EPA Guidance Documents and Memos**
- **Review EPA Rulemaking TSDs**
 - Understand EPA modeling approaches
 - Replicate EPA modeling
- **Participate in Regional Modeling Projects**
 - Conference Calls, Review Technical Reports



IT SUPPORT





SYSTEM ADMINISTRATION

- **Hardware**

- Upgrading/repairing hardware components
- Configuring/connecting disks

- **Operating System**

- User/Group Management (e.g. File Permission)
- Configuring system software
- Installing patches and upgrading operating system
- Network/Security Configuration (e.g., SSH and Firewall)
- Managing licenses for modeling related software (e.g., FORTRAN compiler)

- **Modeling Applications**

- Compiling modeling related software such as IOAPI, CAMx, and CMAQ
- Backup and archiving
- Trouble-shooting

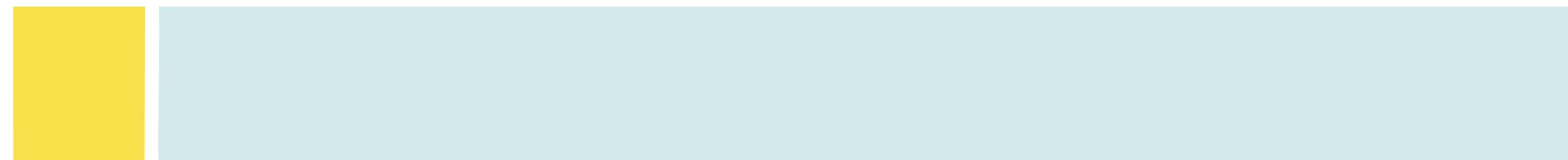


IT SUPPORT OPTIONS

System	Hardware Repairs	Hardware Maintenance	Operating System	Modeling Applications
Leased Server	Contractor	Contractor	Contractor	EPD Staff
Standalone Workstation	Contract (\$1000/3 years)	EPD Staff	EPD Staff	EPD Staff
Cloud Computing	Behind the scenes (N/A)	Vendor	EPD Staff	EPD Staff



EXAMPLE APPLICATIONS





EXAMPLE APPLICATIONS

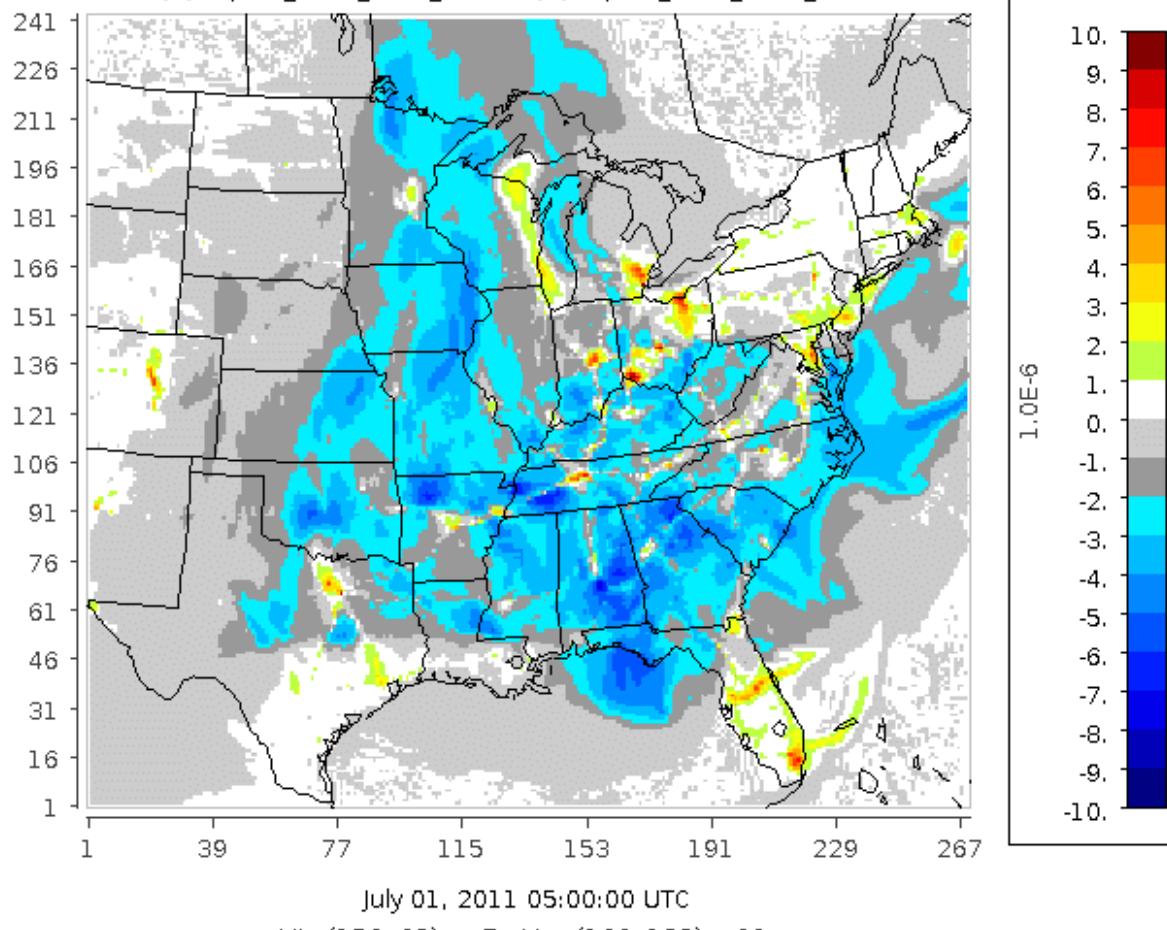
- Ozone projection modeling for attainment SIPs
 - 2008/2015 ozone standards
- Ozone transport modeling for infrastructure SIPs
 - 2008/2015 ozone standards
- Visibility modeling for Regional Haze SIPs
 - Reasonable Progress Goals (RPGs)
- Designation recommendations
 - 2015 ozone standard
- PSD Permit Modeling
 - Secondary PM_{2.5} and ozone impacts (Appendix W)
- Special Projects



50% REDUCTION ON-ROAD NOx

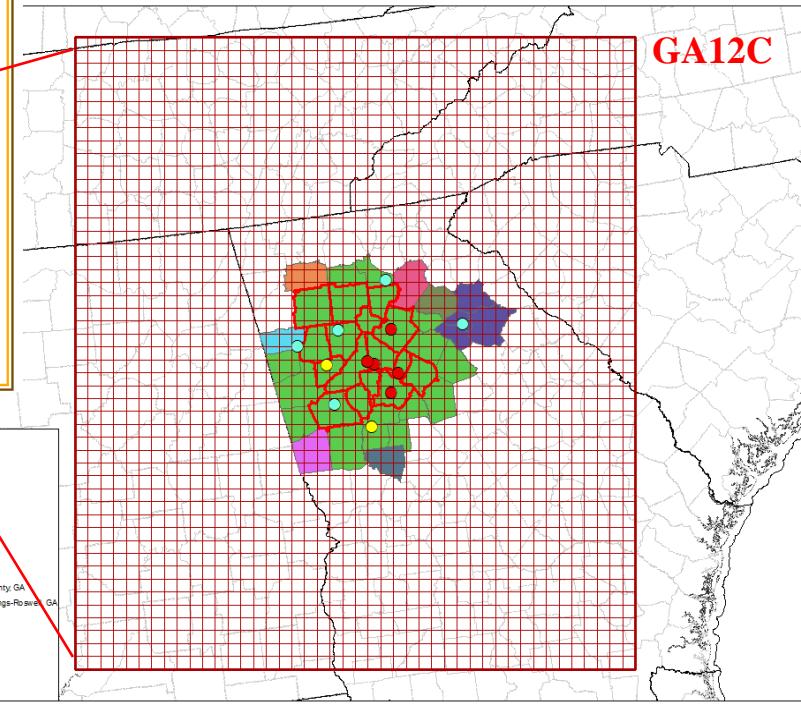
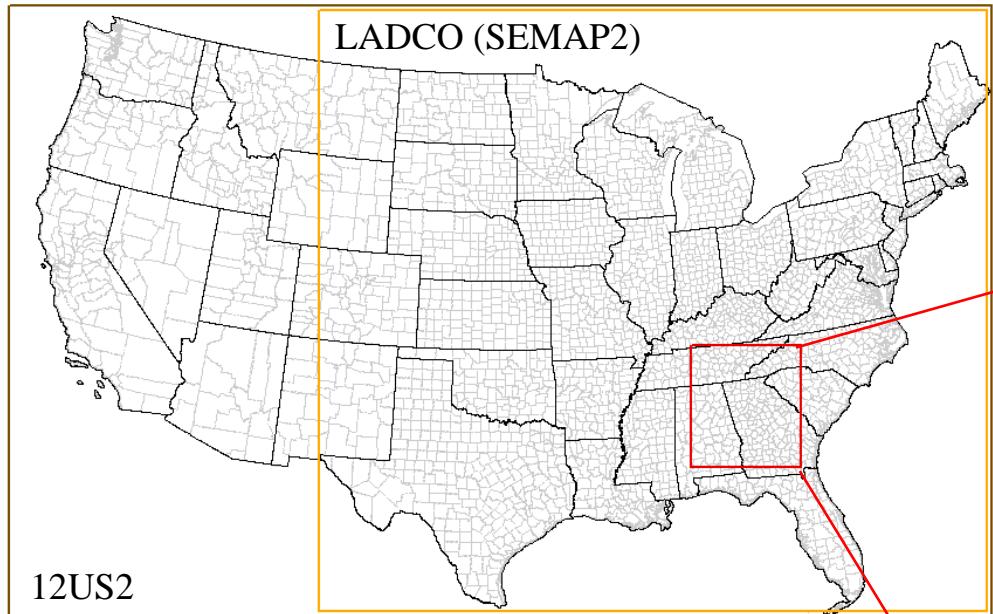
Layer 1 ($O_3[6]-O_3[1]$)*1000.

[1]=epaeef_ram4_base_03.ncf; [6]=epaeef_TR50_ram4_03.ncf





2015 OZONE RECOMMENDATIONS

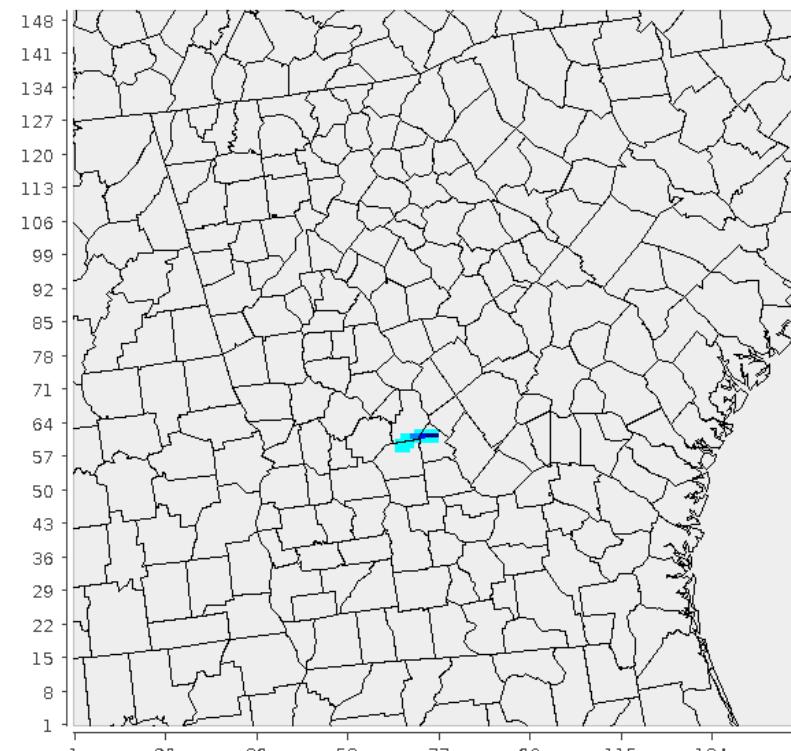




SINGLE SOURCE PSD PERMITTING

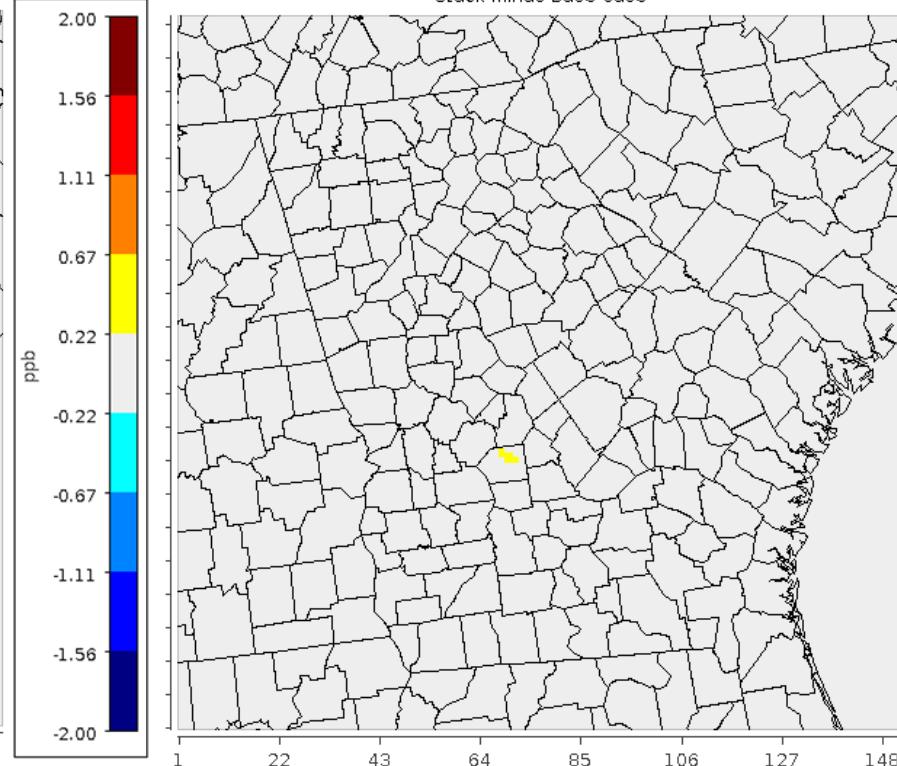
O3

Stack minus Base Case



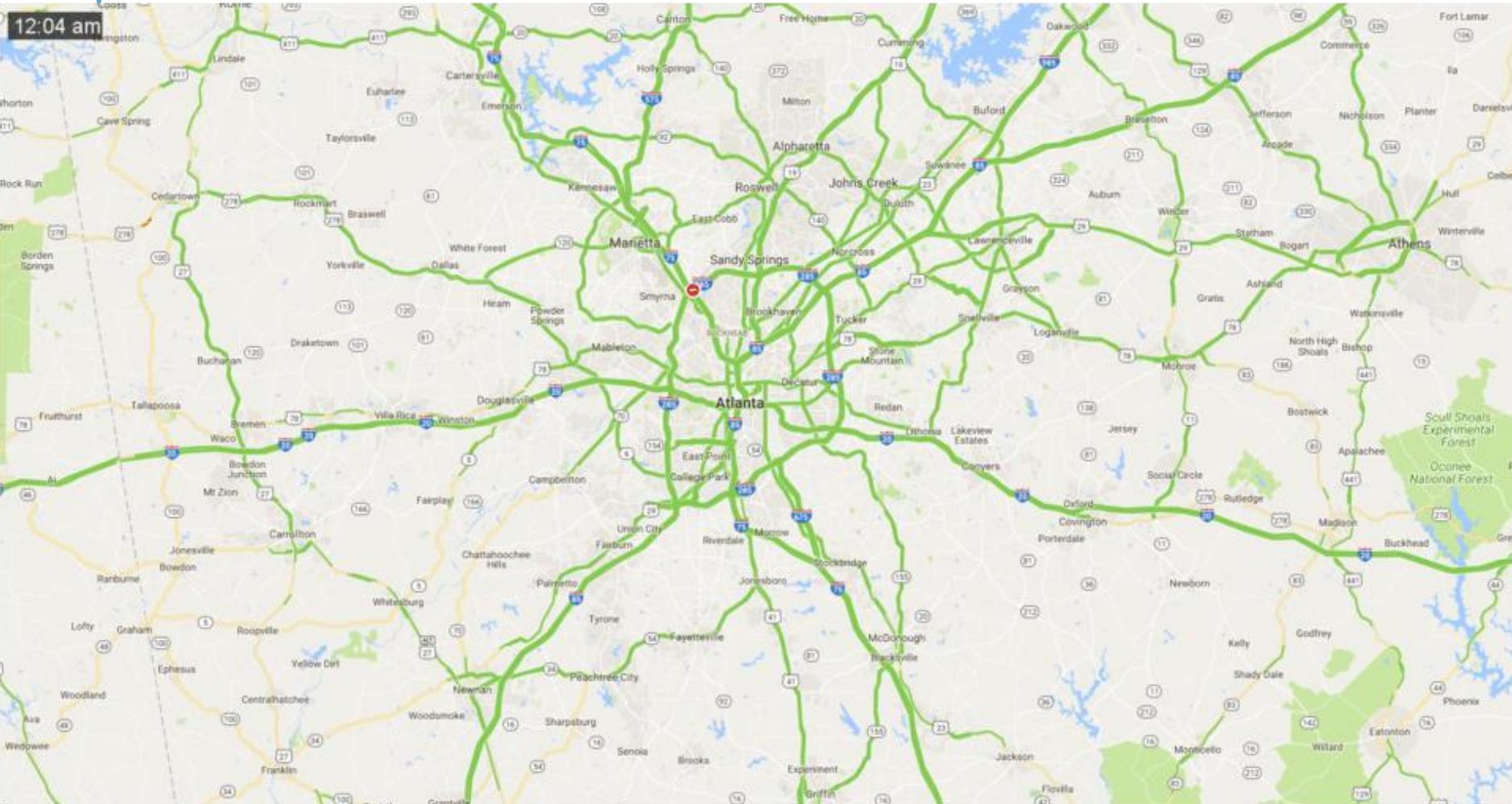
Secondary PM_{2.5}

Stack minus Base Case





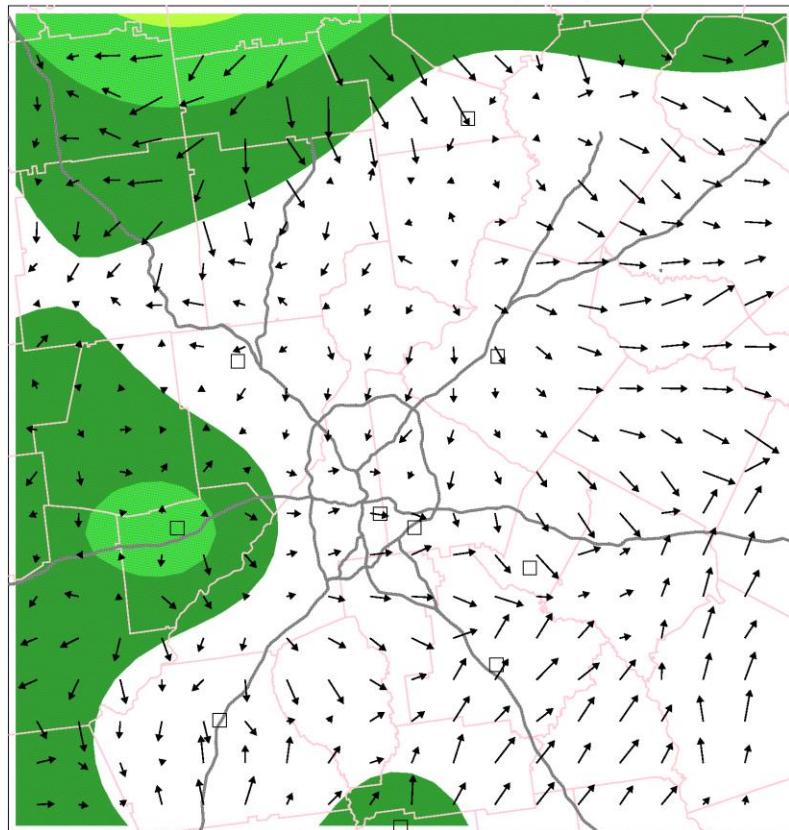
GOOGLE TRAFFIC MAP ON JULY 26



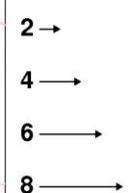
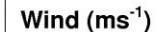
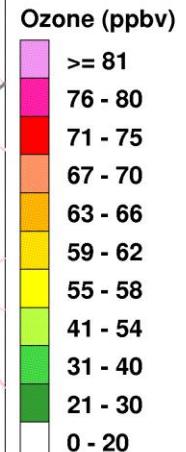
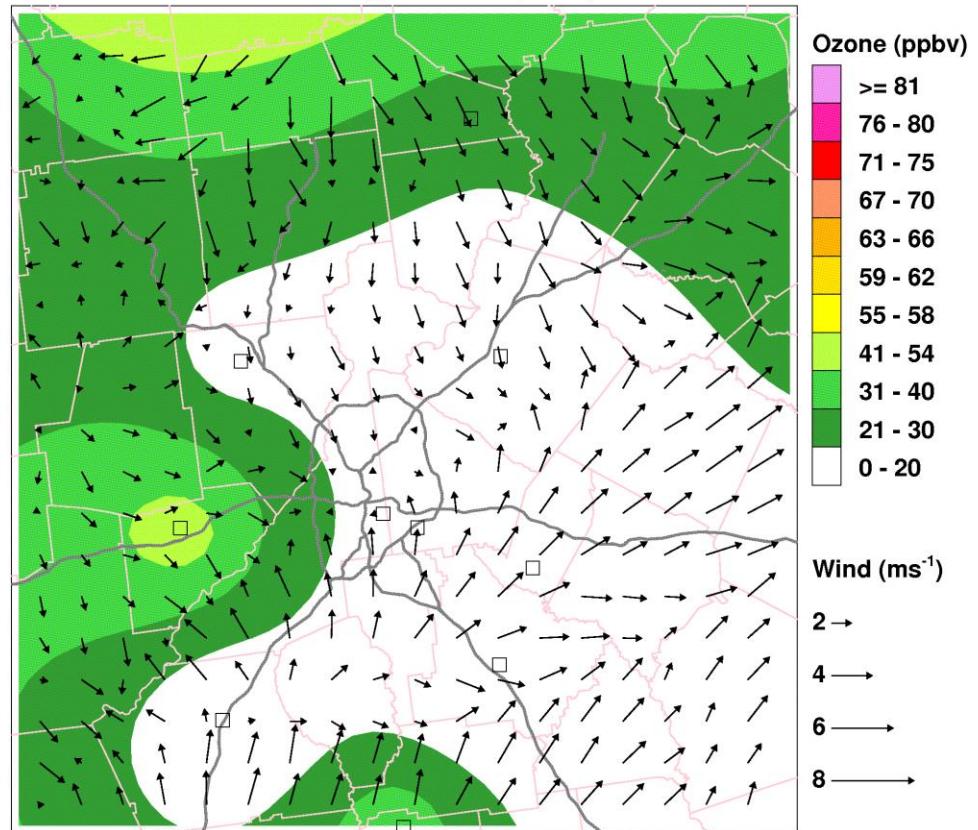


OZONE ANIMATIONS

Surface Ozone & Wind in Metro Atlanta
2017-05-15_00:00:00 (EDT)

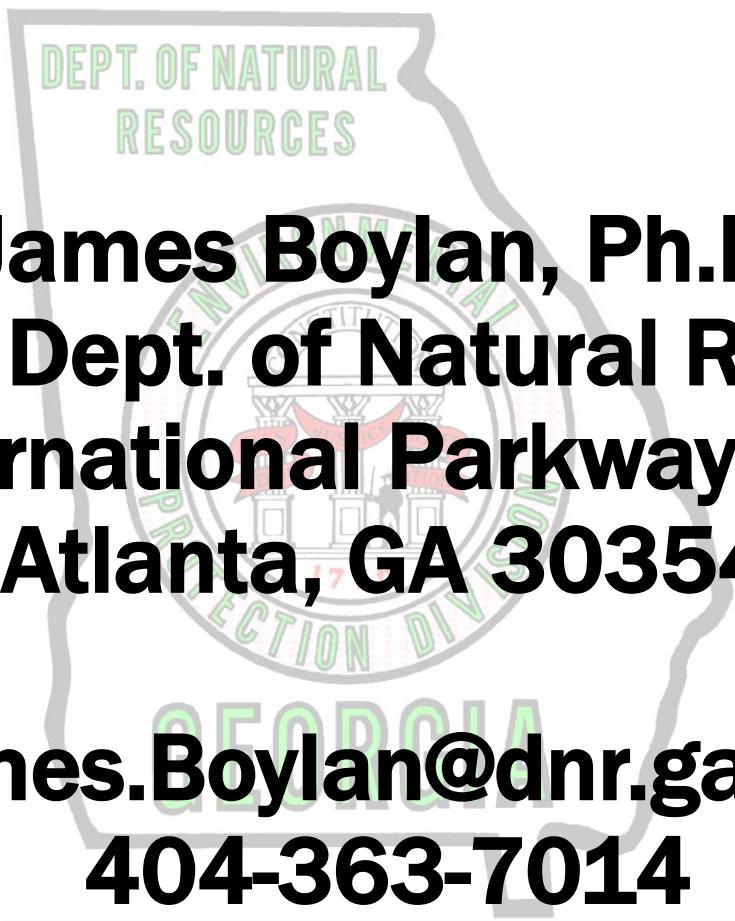


Surface Ozone & Wind in Metro Atlanta
2017-05-16_00:00:00 (EDT)





CONTACT INFORMATION



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