

# THE U.S. EPA COMMUNITY MULTISCALE AIR QUALITY (CMAQ) MODELING SYSTEM –OVERVIEW

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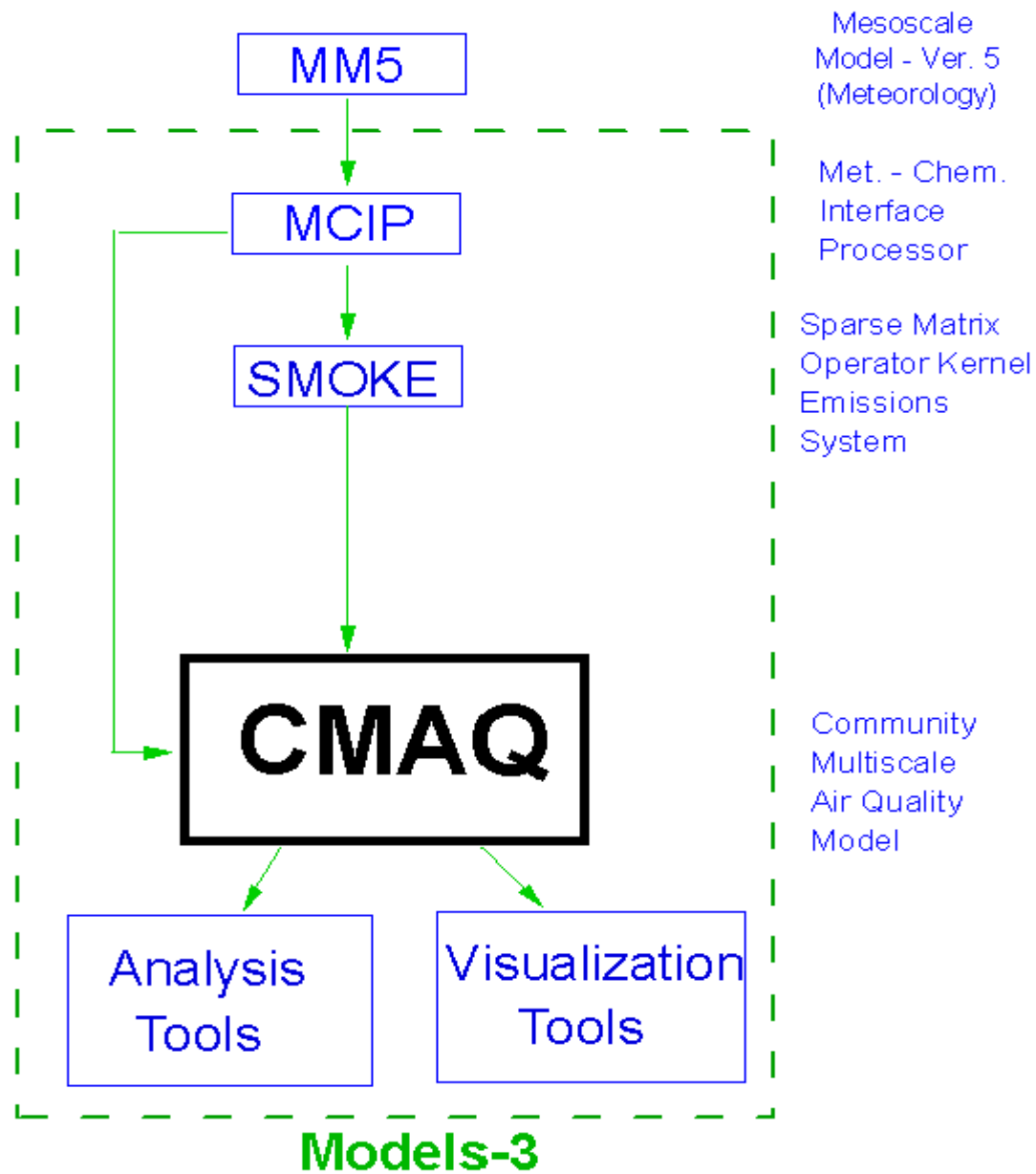
\* On assignment to the National Exposure Research Laboratory, U.S. EPA.

CMAQ Model Peer Review Meeting  
R.T.P., NC  
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*Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.*

# CMAQ Background

- 1970's – Urban Airshed Models
- 1980's – Regional Models
  - Regional Oxidant Model (ROM)
  - Regional Acid Deposition Model (RADM)
    - Driven by MMx meteorological model
- 1990's
  - Multiscale Model
    - Community Multiscale Air Quality Model (CMAQ)
      - MM5 meteorology model, SMOKE emissions model
      - 1998- first public release; annual releases since



# CMAQ Chemical Transport Model

## *September 2003 Release*

- Advection
  - Piecewise parabolic method (PPM)
  - Bott scheme
  - *Layer-dependent horizontal advection time-stepping*
- Vertical Diffusion
  - Eddy-diffusivity ( $K_z$ )
  - Asymmetric Convective Model (ACM)
- Horizontal Diffusion
  - Eddy-diffusivity with  $K_h$  grid size dependent

- Cloud Processes

- Aqueous chemistry and sub-grid clouds adapted from RADM
- Simple grid-resolved cloud scheme at all grid resolutions
- *Updates to Henry's Law constants (Seinfeld and Pandis, 1998)*
- *New timestep calculation in aqueous chemistry process*
- *Revisions to washout of coarse model aerosol number concentration*
  - *Preserves aerosol diameter during the washout process*

- Plume in Grid
  - Embedded Lagrangian plume with gas-phase photochemistry (*aerosols now being added – in 2004 model release*)
- Dry deposition
  - RADM dry deposition model
  - M3dry: Adjunct to the PX Land Surface Model

- Gas-phase Chemical Mechanisms
  - RADM2
  - CB4
  - SAPRC99
  - All mechanisms linked to aerosol module and aqueous chemistry
  - $N_2O_5 + H_2O \rightarrow 2HNO_3$ 
    - *Eliminated gas-phase rxn from all mechanisms by zeroing rate constant (defer to heterogeneous pathway)*
  - *Eliminated advection/diffusion of fast-reacting species (CB4-only)*

- Gas-phase Chemistry Solvers
  - Quasi-steady state approximation (QSSA)
  - SMVGEAR
  - Modified Euler Backward Iterative (MEBI) method for all mechanisms
  - *Euler Backward Iterative (EBI) gas-phase chemistry solver for CB4*



# Aerosol Model (Aero3)

- Lognormal size distribution ( $\sigma_g$  and  $D_g$ )
  - Aitken mode (0-0.1  $\mu\text{m}$ )
  - Accumulation mode (0.1-2.5  $\mu\text{m}$ )
  - Coarse (PM10 - PM2.5)
- Aerosol processes:
  - Nucleation
  - Coagulation
  - ISORROPIA semivolatile equilibrium model
  - Clouds - CCN, aqueous chemistry, wet deposition

- Aerosol chemistry
  - Inorganic: Sulfate, Nitrate, Ammonium
  - Secondary anthropogenic and biogenic organic
    - *SOA algorithm modified to make the gas-particle partitioning reversible*
    - *Eliminated SOA production from anthropogenic alkenes*
    - *Adjusted yields of semi-volatiles from alkanes and aromatics*
    - *Modified gas-phase monoterpene reaction rates in RADM2 and CB4*

– Speciated primary emissions

- Elemental carbon, organic carbon, sulfate, nitrate
- *Future: wildfire emissions, soil and fugitive dust, sea salt*

– Heterogeneous reaction of  $\text{N}_2\text{O}_5 \rightarrow \text{HNO}_3$

- *Modified reaction probability based on Riemer (2003)*

- Regional haze

– Visibility estimates in deciviews

$$\text{deciView} = 10 \ln (\beta_{\text{ext}} / 0.01)$$

- Meteorology Chemistry Interface Processor (MCIP2)
  - MM5v3 compatible
  - Surface and PBL parameters passed through
  - Compatible w/ PX LSM and M3dry
  - *Updates for wintertime conditions; effects of snow cover on deposition*
  - *New dry deposition species: N<sub>2</sub>O<sub>5</sub>, NO<sub>3</sub>, aldehydes*
- Emissions
  - Sparse Matrix Operator Kernel Emissions (SMOKE)
  - Biogenic Emissions Inventory System (BEIS3)

- *Change in order of time-splitting science processes*

*Previous Order*

*advection*

*mass adjustment*

*horiz. diffusion*

*vert. diffusion*

*clouds*

*chemistry*

*aerosols*

*New Order*

*vertical diffusion*

*advection*

*mass adjustment*

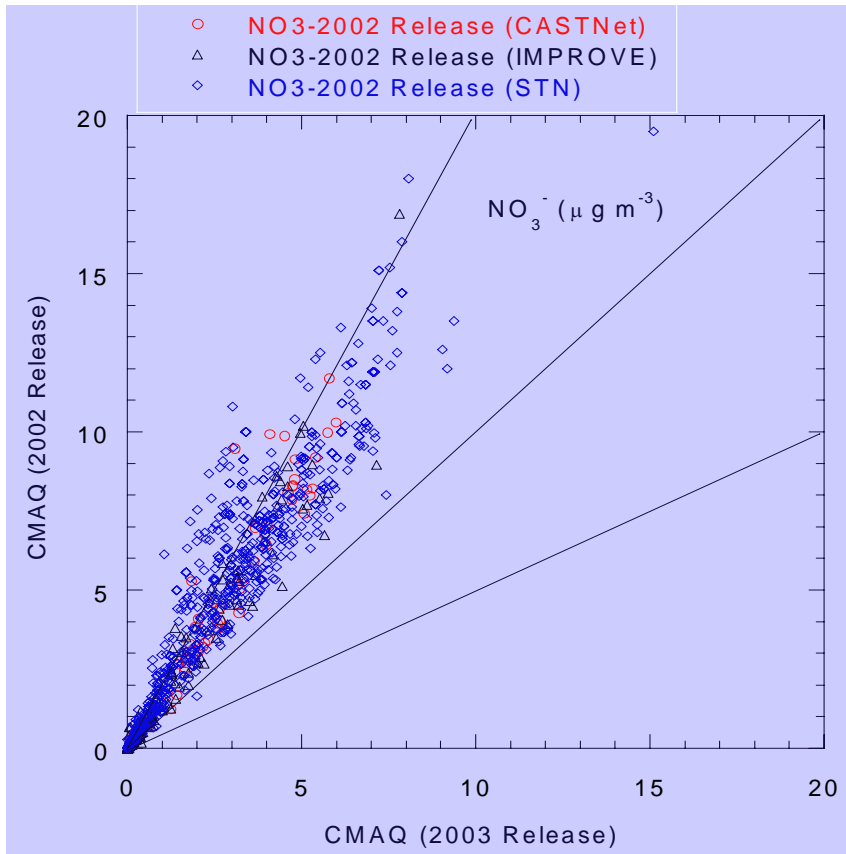
*horiz. diffusion*

*clouds*

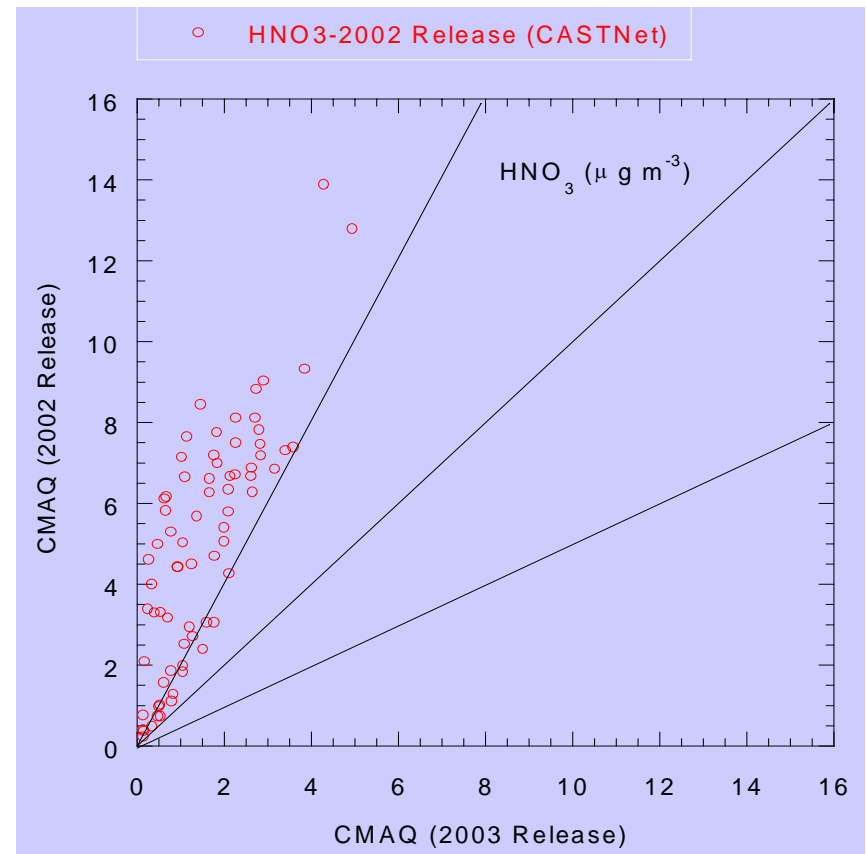
*chemistry*

*aerosols*

# 2003 release vs 2002 release



Aerosol Nitrate



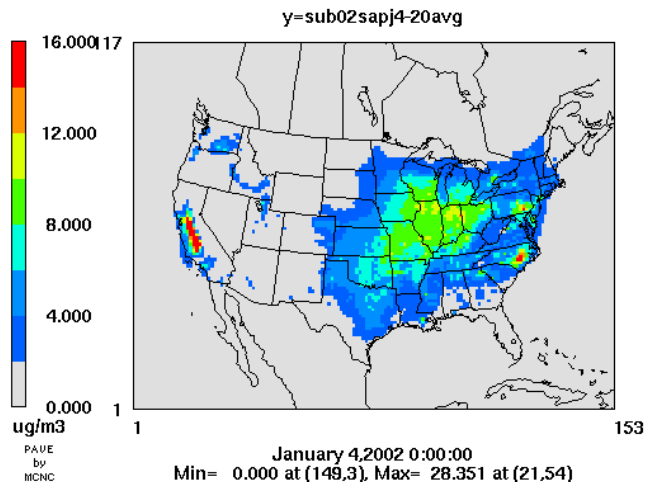
Gas Phase Nitric Acid

January 4 – 20, 2002

# CMAQ02 vs CMAQ03 - Nitrate

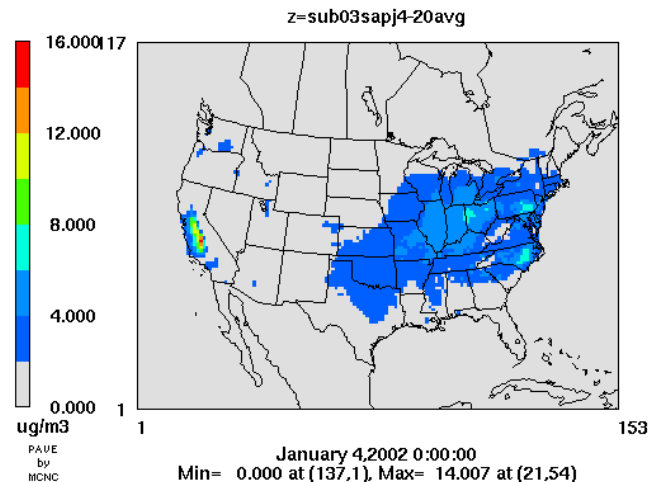
Layer 1 ANO3Ty

Nitrate  
Aerosol  
CMAQ02



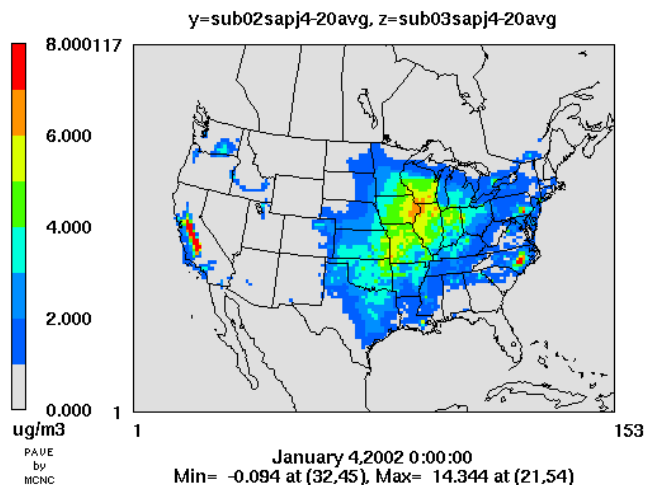
Layer 1 ANO3Tz

Nitrate  
Aerosol  
CMAQ03



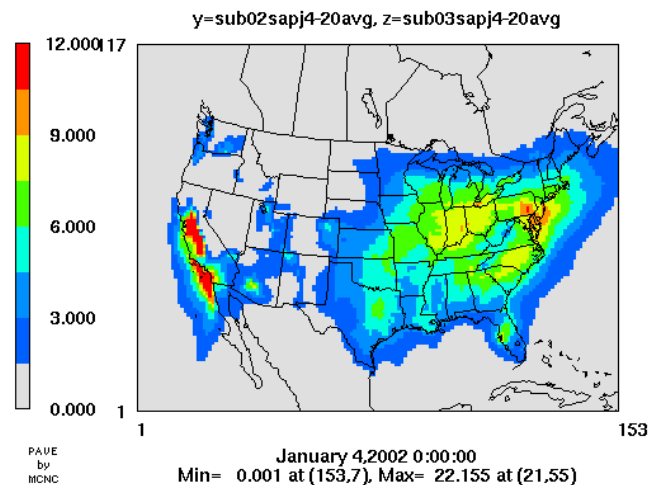
Layer 1 ANO3Ty-ANO3Tz

Nitrate  
Aerosol  
diff



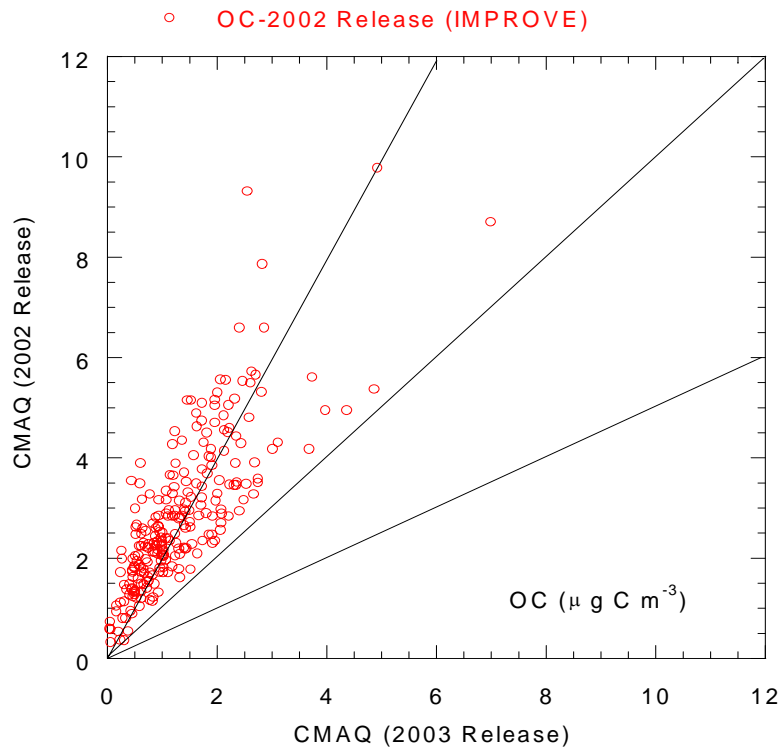
Layer 1 ANO3Ty+2835\*(HNO3y-HNO3z)-ANO3'

Total  
Nitrate  
diff

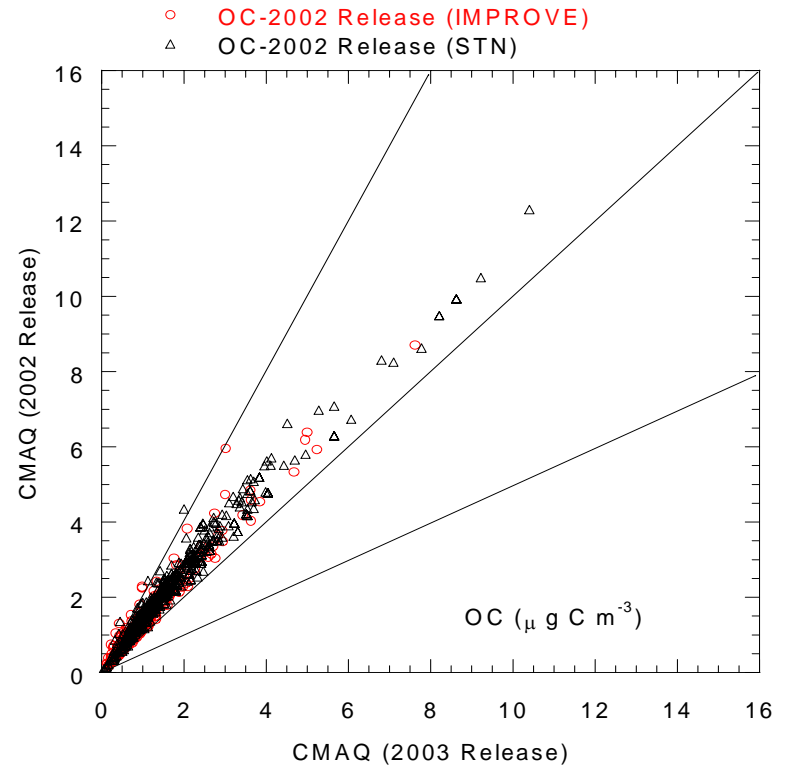


Average concentrations January 4 – 20, 2002

# Organic Carbon Aerosol



June 15 – 29, 1999



Jan. 4 - 20, 2002

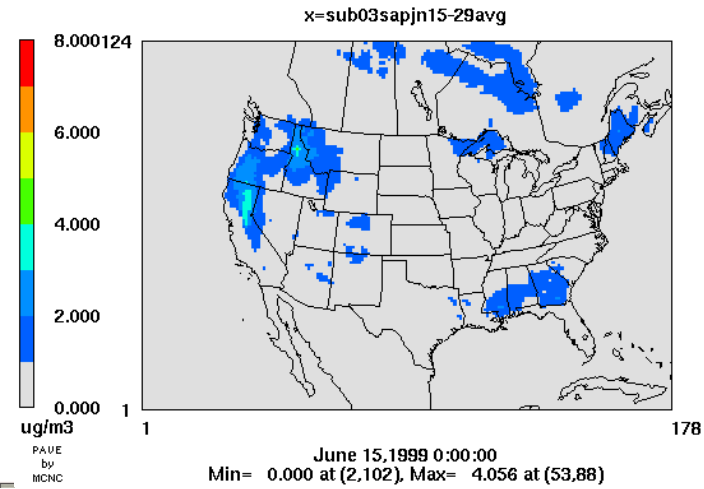
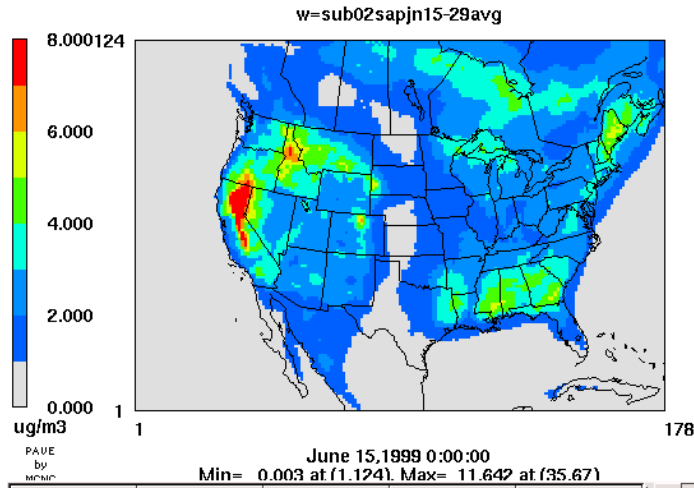


# CMAQ02 vs CMAQ03 - SOA

Layer 1 AORGATw+AORGBTw

Layer 1 AORGATx+AORGBTx

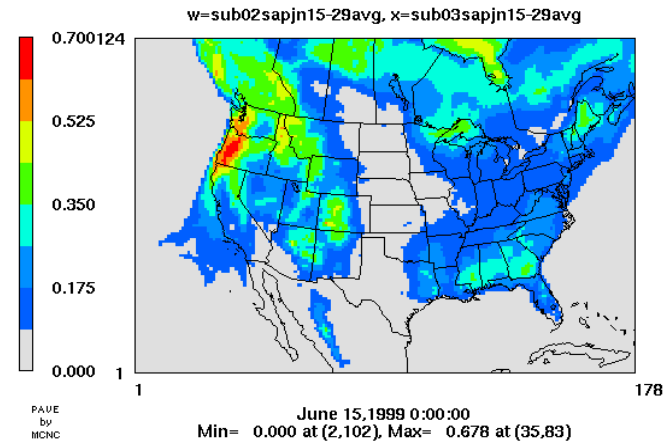
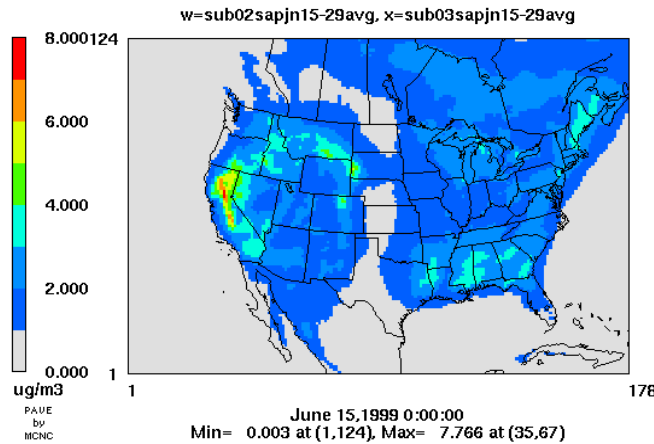
Total SOA CMAQ02



Total SOA CMAQ03

ayer 1 (AORGATw+AORGBTw)-(AORGATx+AORGBTx)/(AORGATw+AORGBTw)

Total SOA diff



Total SOA Ratio: 03/02

Average concentrations June 15 – 29, 1999

# Outreach

- Community Modeling and Analysis (CMAS) Center at UNC-CH/CEP
  - User support
  - Training
  - Help desk
  - Annual Workshop
  - Support for CMAQ model public releases
  - Web site and electronic resources