

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

Kenneth Schere*

Atmospheric Sciences Modeling Division
NOAA - Air Resources Laboratory
Research Triangle Park, NC

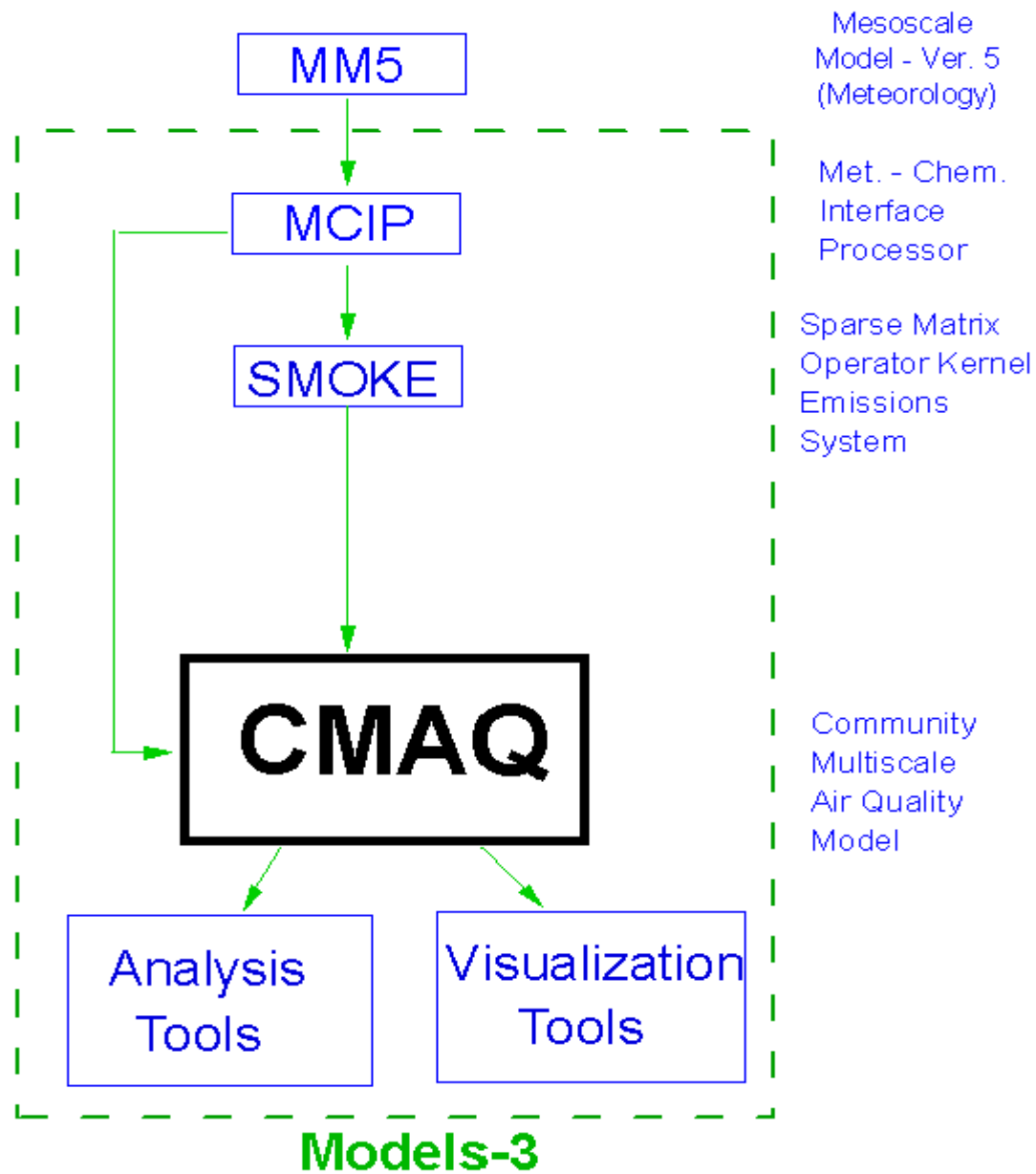
* On assignment to the National Exposure Research Laboratory, U.S. EPA.

CMAQ Model Peer Review Meeting
R.T.P., NC
December 17, 2003

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 (σ_g and D_g)
 - Aitken mode (0-0.1 μm)
 - Accumulation mode (0.1-2.5 μm)
 - 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: N₂O₅, NO₃, 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

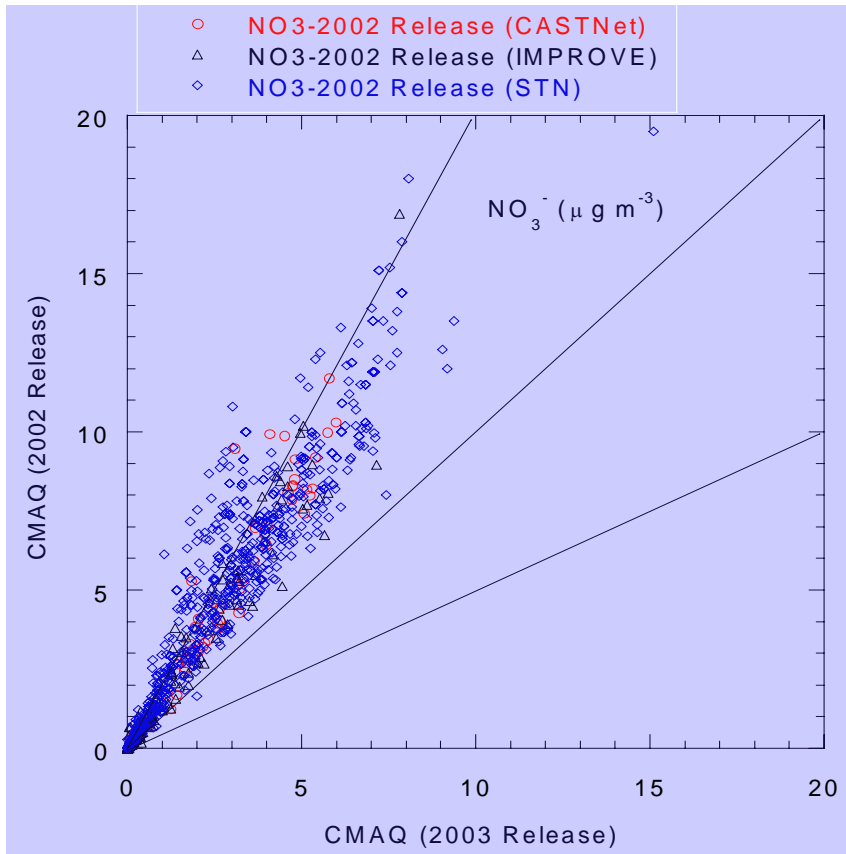
horiz. diffusion

clouds

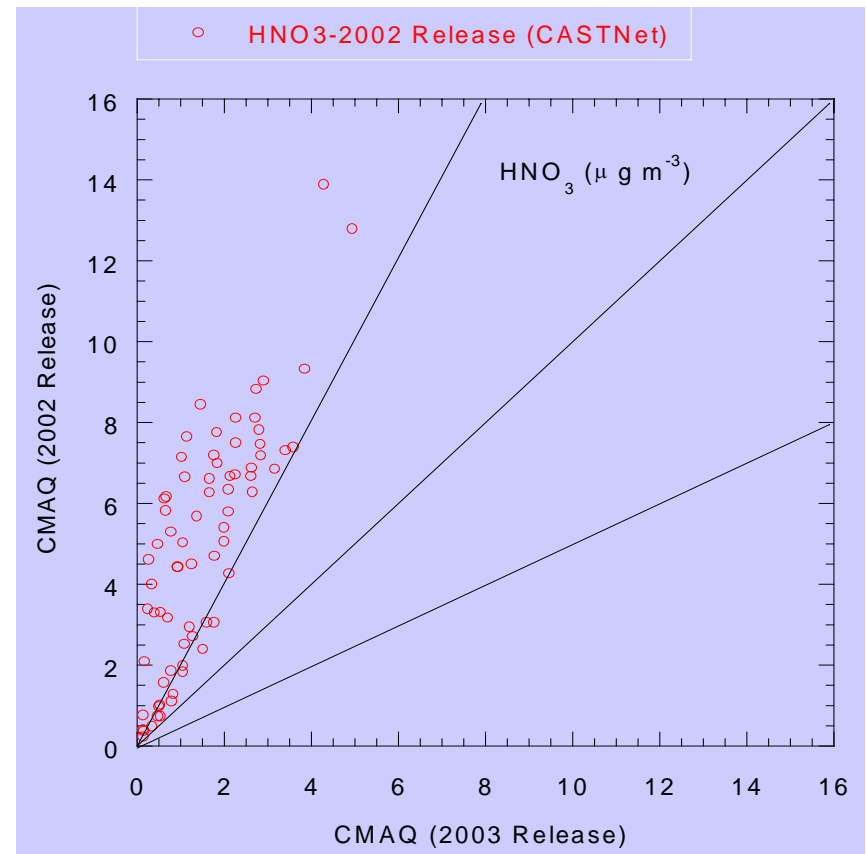
chemistry

aerosols

2003 release vs 2002 release



Aerosol Nitrate



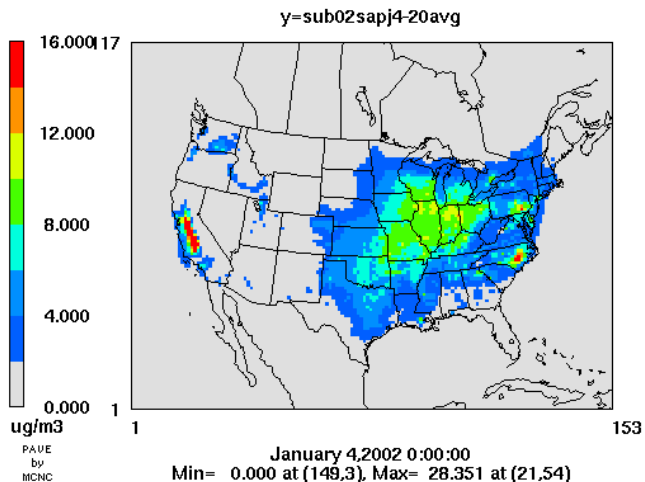
Gas Phase Nitric Acid

January 4 – 20, 2002

CMAQ02 vs CMAQ03 - Nitrate

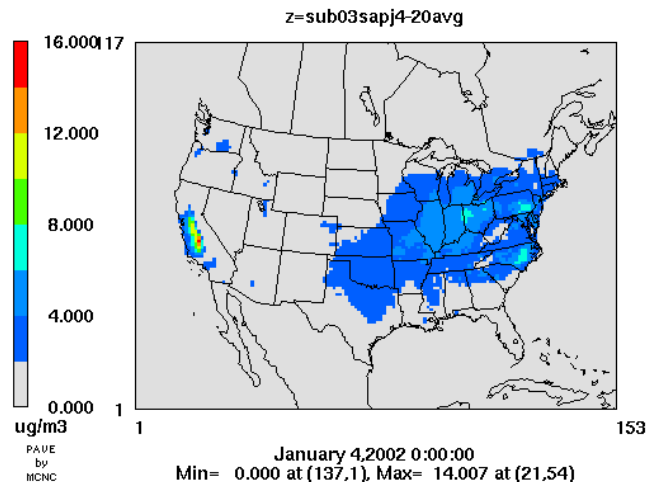
Layer 1 ANO3Ty

Nitrate
Aerosol
CMAQ02



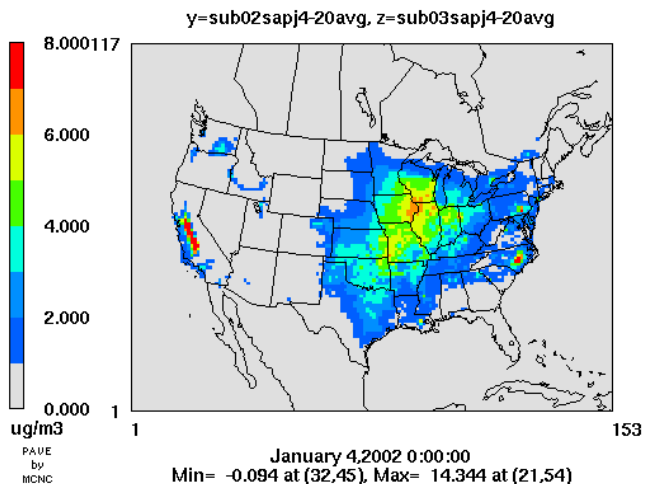
Layer 1 ANO3Tz

Nitrate
Aerosol
CMAQ03



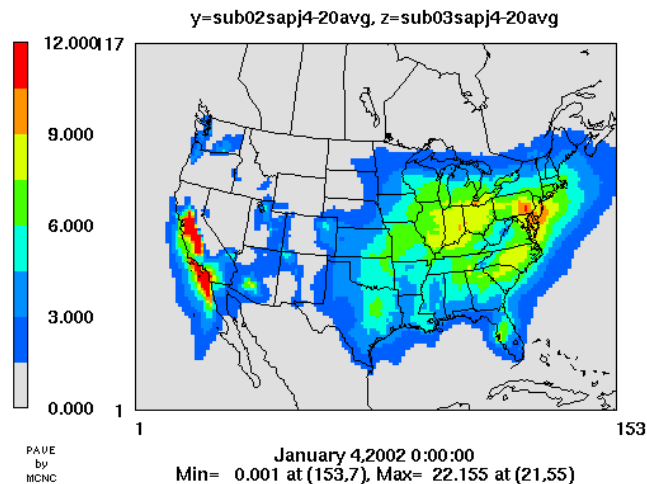
Layer 1 ANO3Ty-ANO3Tz

Nitrate
Aerosol
diff



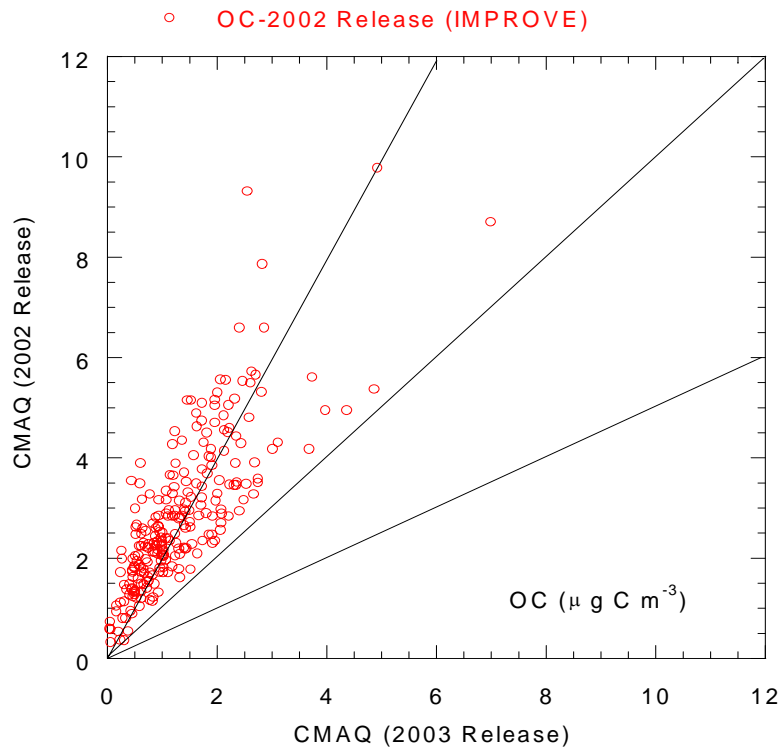
Layer 1 ANO3Ty+2835*(HNO3y-HNO3z)-ANO3'

Total
Nitrate
diff

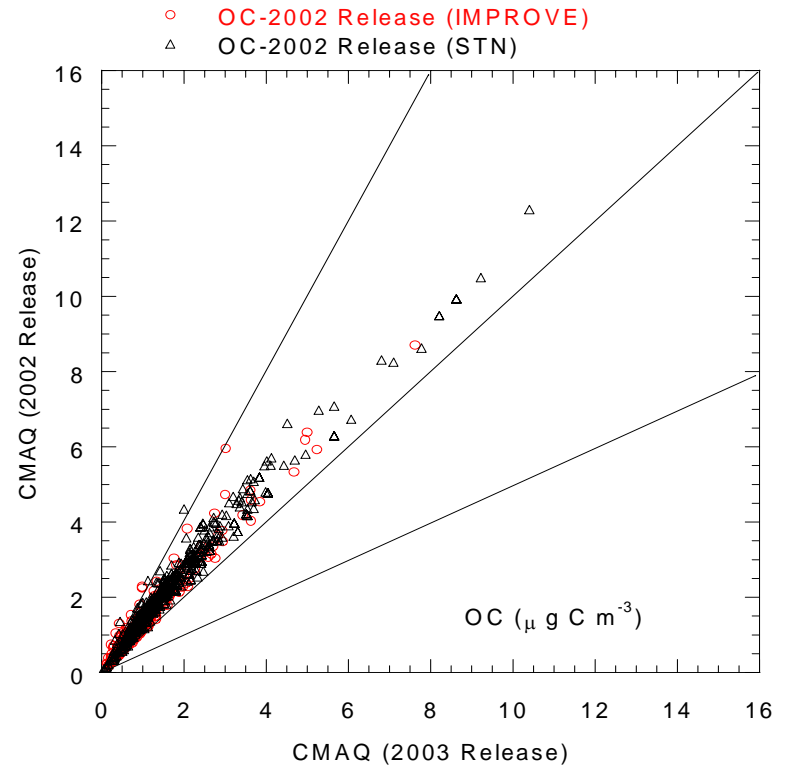


Average concentrations January 4 – 20, 2002

Organic Carbon Aerosol



June 15 – 29, 1999



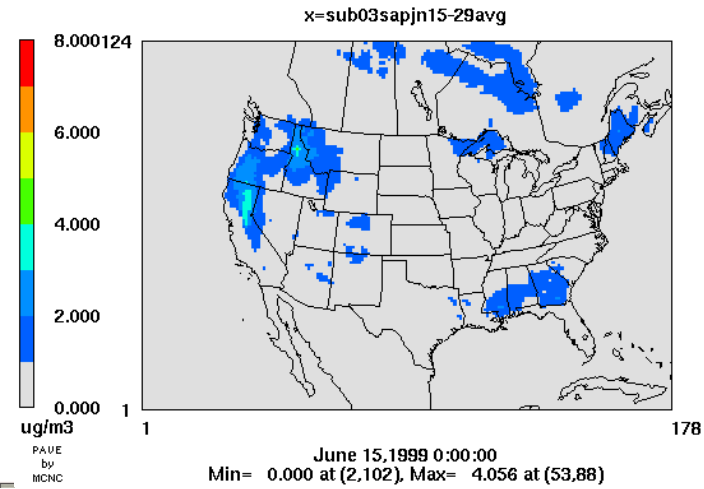
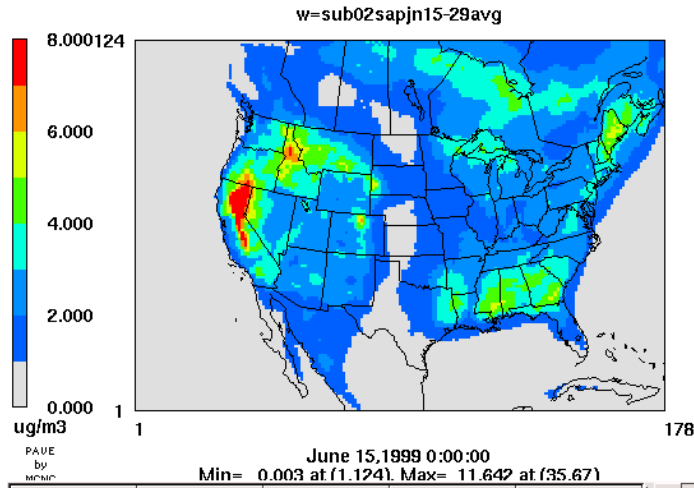
Jan. 4 - 20, 2002

CMAQ02 vs CMAQ03 - SOA

Layer 1 AORGATw+AORGBTw

Layer 1 AORGATx+AORGBTx

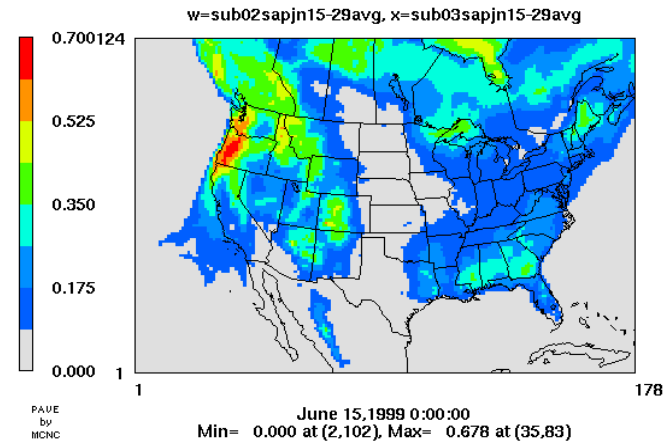
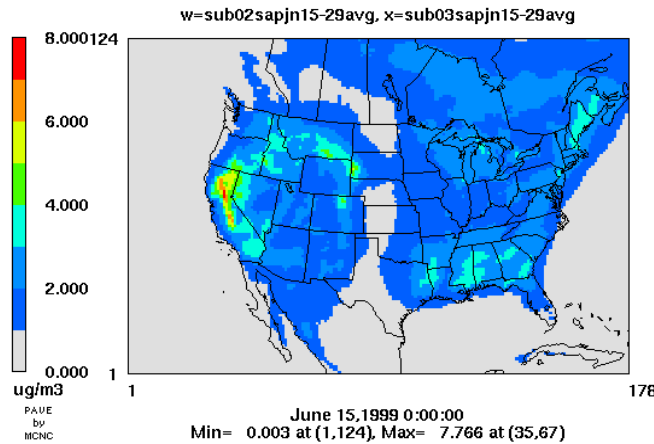
Total SOA CMAQ02



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