New Developments in CMAQ Model Physics

Jonathan Pleim, Shawn Roselle, Jeffrey Young, Donna Schwede, Rohit Mathur, Prakash Bhave
and the CMAQ Model Development Team
Atmospheric Sciences Modeling Division, NOAA
RTP, NC

New Features in CMAQv4.5

- Physical Processes (main focus of this talk)
- Aerosols (see Prakash Bhave's Poster)
  - Sea salt (see Uma Shankar's Poster)
  - PM2.5 size cut
  - Updates to ISORROPIA
  - Aerosol module bug fixes
- Gas-Phase Chemical Processes
  - Toxics – subset of HAPs
  - Chlorine chemistry – added to CB4
- Tools
  - Carbon source apportionment
  - Sulfur tracking

CMAQ Model Physics

- Mass Conservation
- Minimum eddy diffusivity
- Aerosol Dry Deposition
- Convective Clouds

Mass Conservation

- MM5/CMAQ is a non-hydrostatic, compressible, off-line model system
- Must correct advection results for inconsistencies in Mass and Momentum fields caused by:
  - Interpolations (time and space)
  - Inaccuracies in MM5 (not mass conserving)
  - Numerical errors
- Previous Releases:

$$c_i J_s = \frac{(c_i J_s)^T}{(\rho_a J_s)^T} (\rho_a J_s)^{met}$$

$$J_s = \frac{\partial z}{\partial s}$$

New scheme for mass continuity (v4.5)

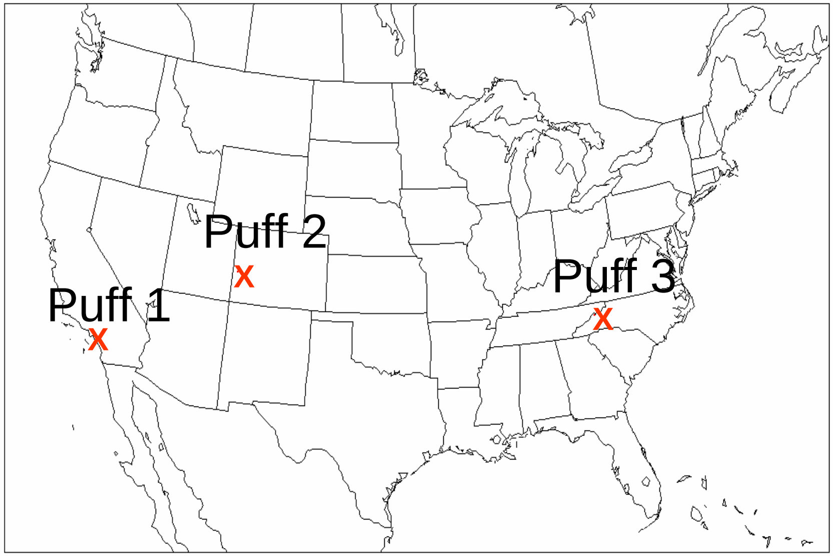
- Mass Continuity: $\frac{\partial \rho J}{\partial t} = -\nabla \bullet (\rho J\mathbf{V})$

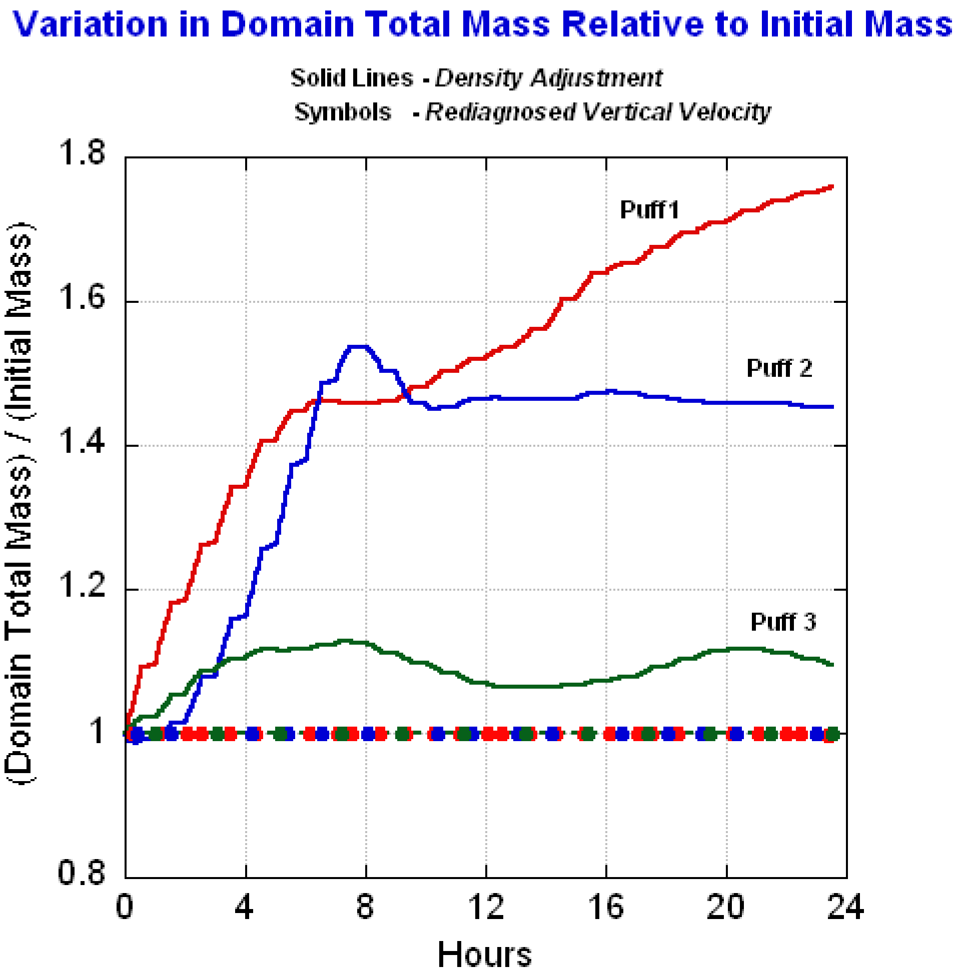
1. Advect in X and Y including cross error correction
2. Solve for w_k starting at surface $w_{sfc} = 0$

$$w_k = \frac{1}{(\rho J)^{xy}}\left(F_k - F_{k-1}\right)$$

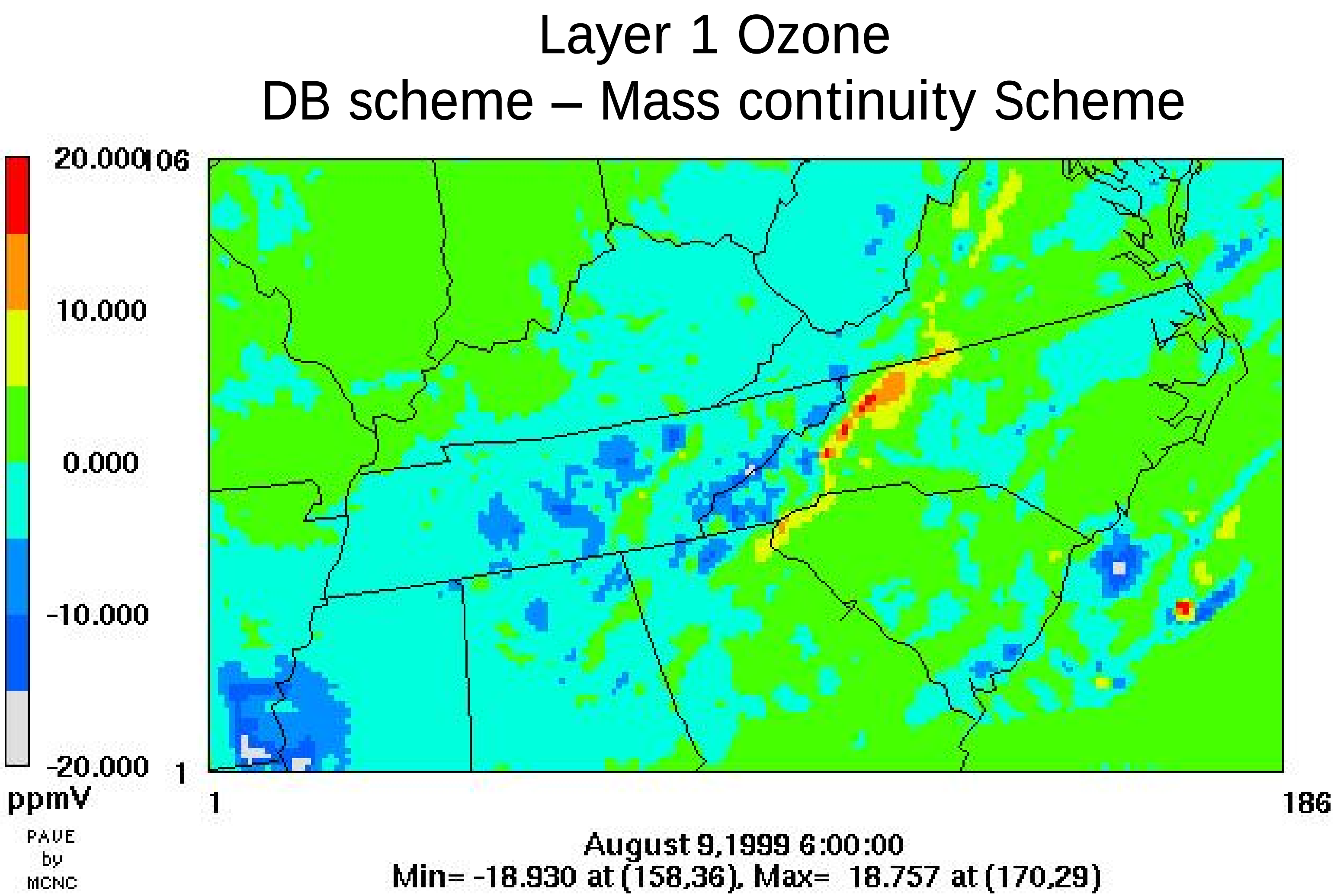
$$F_k = \left((\rho J)^{xy} - (\rho J)^{met}\right)\frac{\Delta z}{\Delta t}$$

Tracked total domain mass of three puffs





Comparison of mass continuity schemes



New minimum K_z

- Previously K_{zmin} = 1.0 m^2/s
- New scheme sets K_{zmin} according to fraction of urban LU category:

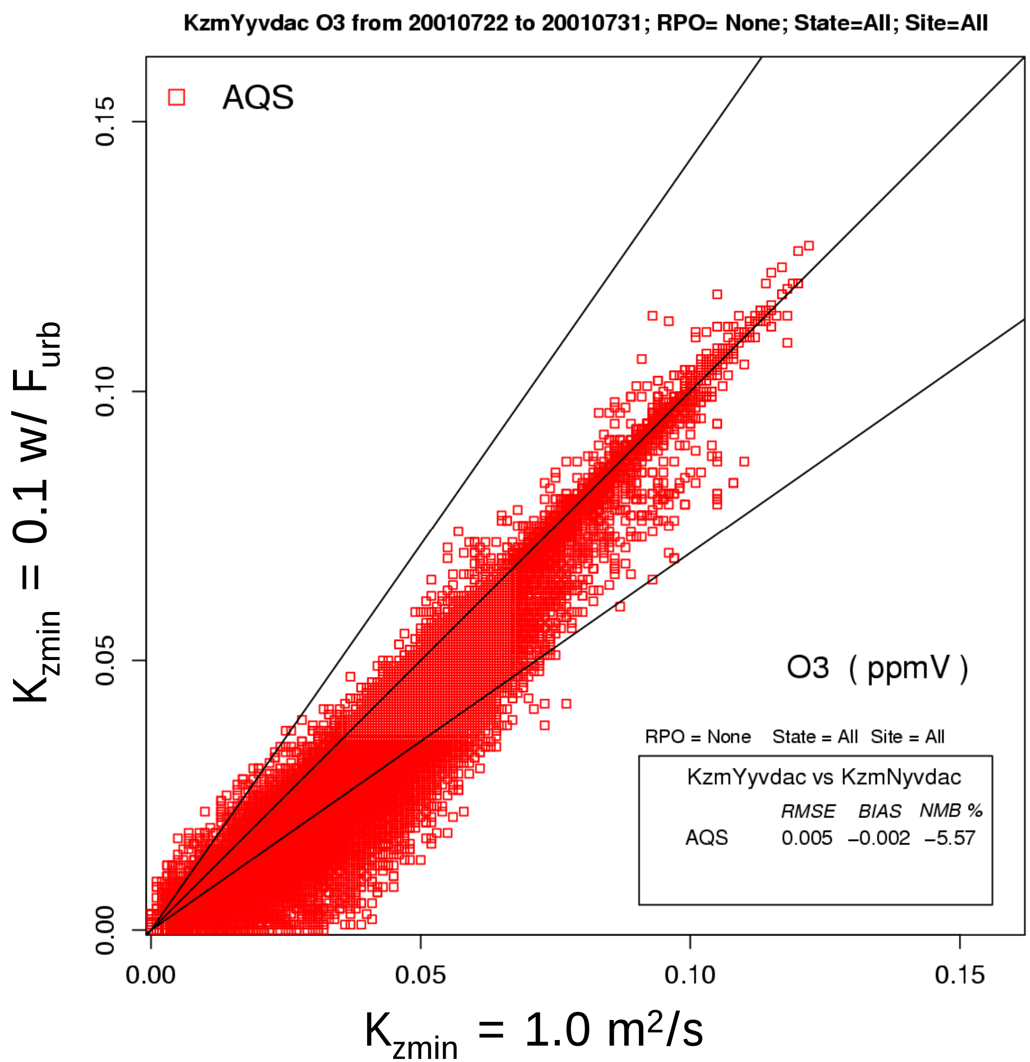
$$K_{z\min} = K_{z\min u} F_{urb} + K_{z\min r}(1 - F_{urb})$$

where $K_{z\min u}$ = 2.0, $K_{z\min r}$ = 0.1 or 0.5 m^2/s

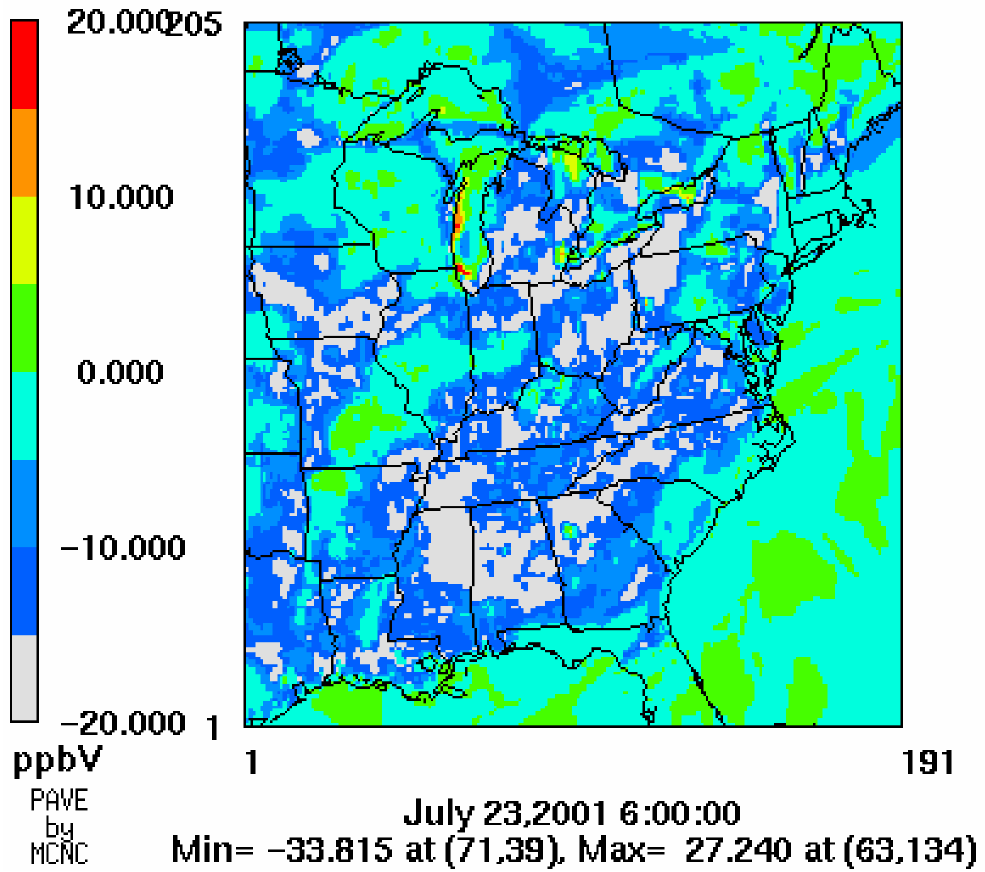
  - Higher urban K_{zmin} is meant to represent reduced nocturnal stability due to urban heat island effects

- Nighttime ozone concentrations much improved
- Primary concentrations much higher in rural areas such as biogenic organics

Effects of minimum K_z on O_3

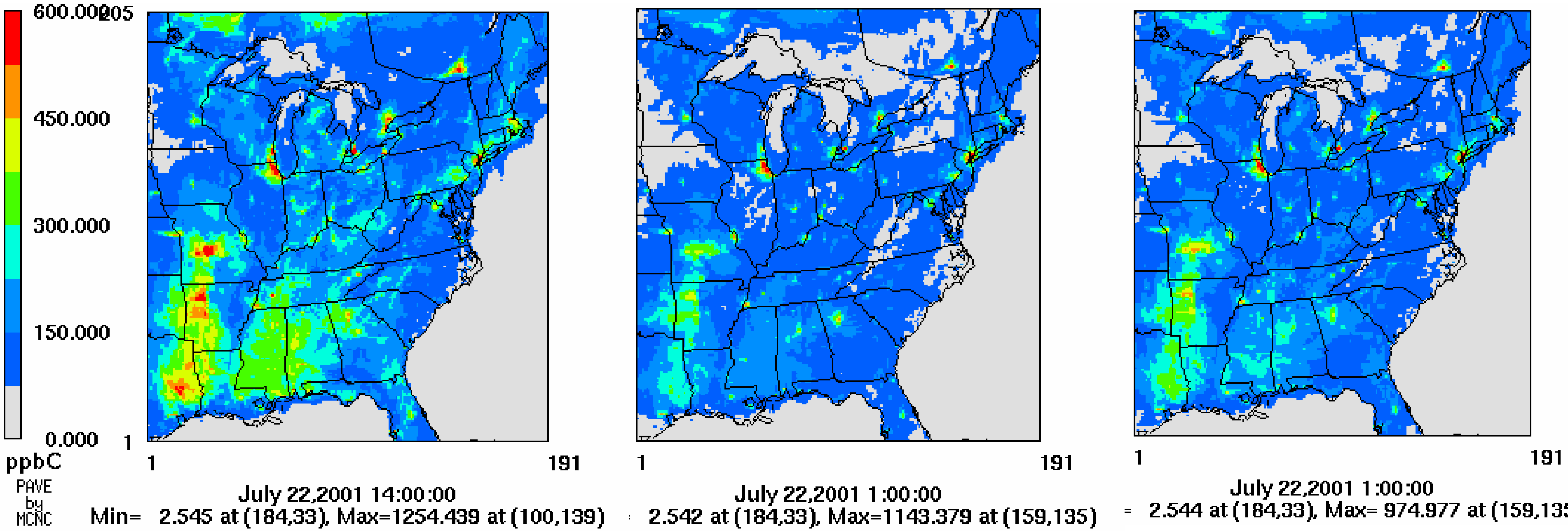


Difference in nocturnal O_3 due to minimum K_z

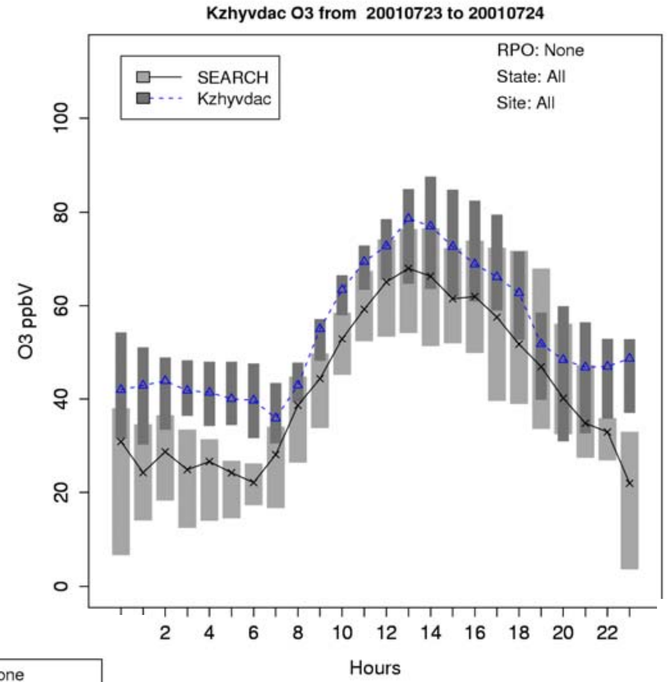


Maximum VOC (ppbC) over 10 day period in July 2001

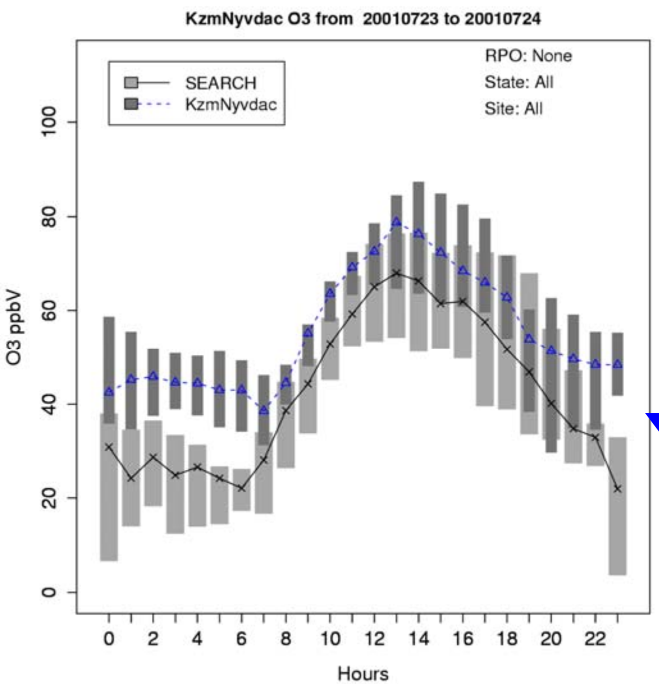
$K_{zmin} = 0.1$ w/ F_{urb} | $K_{zmin}=1.0$ | $K_{zmin} = 0.5$ w/ F_{urb}



Diurnal avg box plots for Search sites – July 23-24

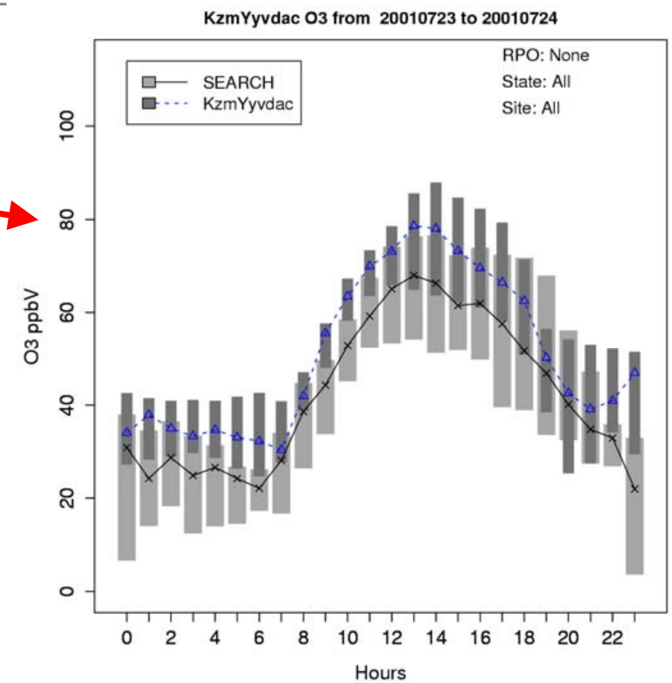


K_{zmin} =0.5 with F_{urb}



K_{zmin} =0.1 with F_{urb}

K_{zmin} =1.0



Aerosol dry deposition modifications

$$v_d = \left[R_a + R_b + R_a R_b v_g\right]^{-1} + v_g$$

Replaced with

$$v_d = \frac{v_g}{\left(1 - \exp(-v_g (R_a + R_b))\right)}$$

Venkatram and Pleim (1999)

Quasi-laminar boundary layer resistance

$$R_b = \left[v(Sc^{-2/3} + E_{im})\right]^{-1} where \qquad v = u_* \left(1 + 0.24 \frac{w_*^{\,2}}{u_*^{\,2}}\right)$$

Impaction term

$$E_{im} = 10^{-3/St}$$

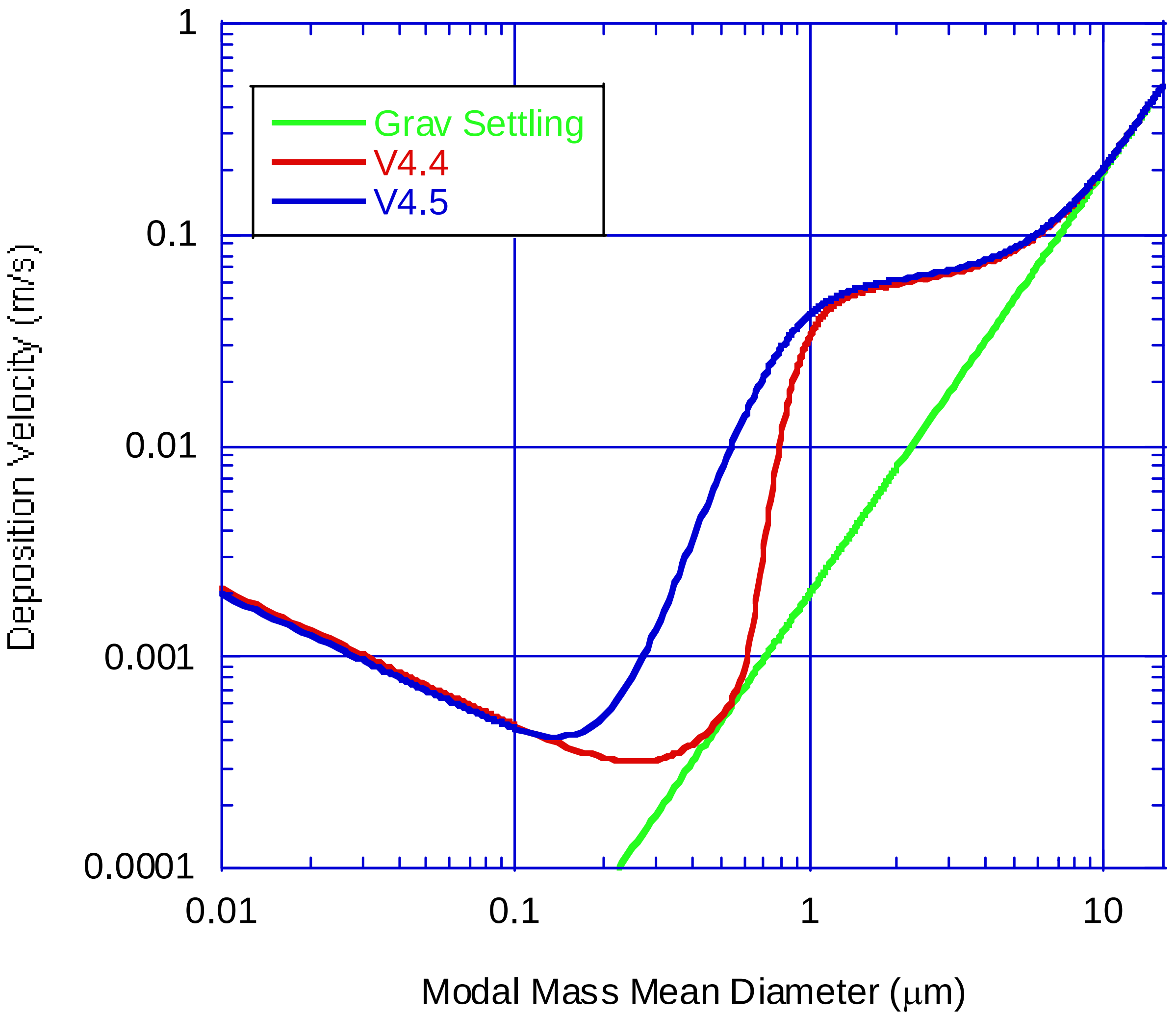
Slinn (1982)

$$E_{im} = \frac{St^2}{400 + St^2} \approx \frac{St^2}{400}$$

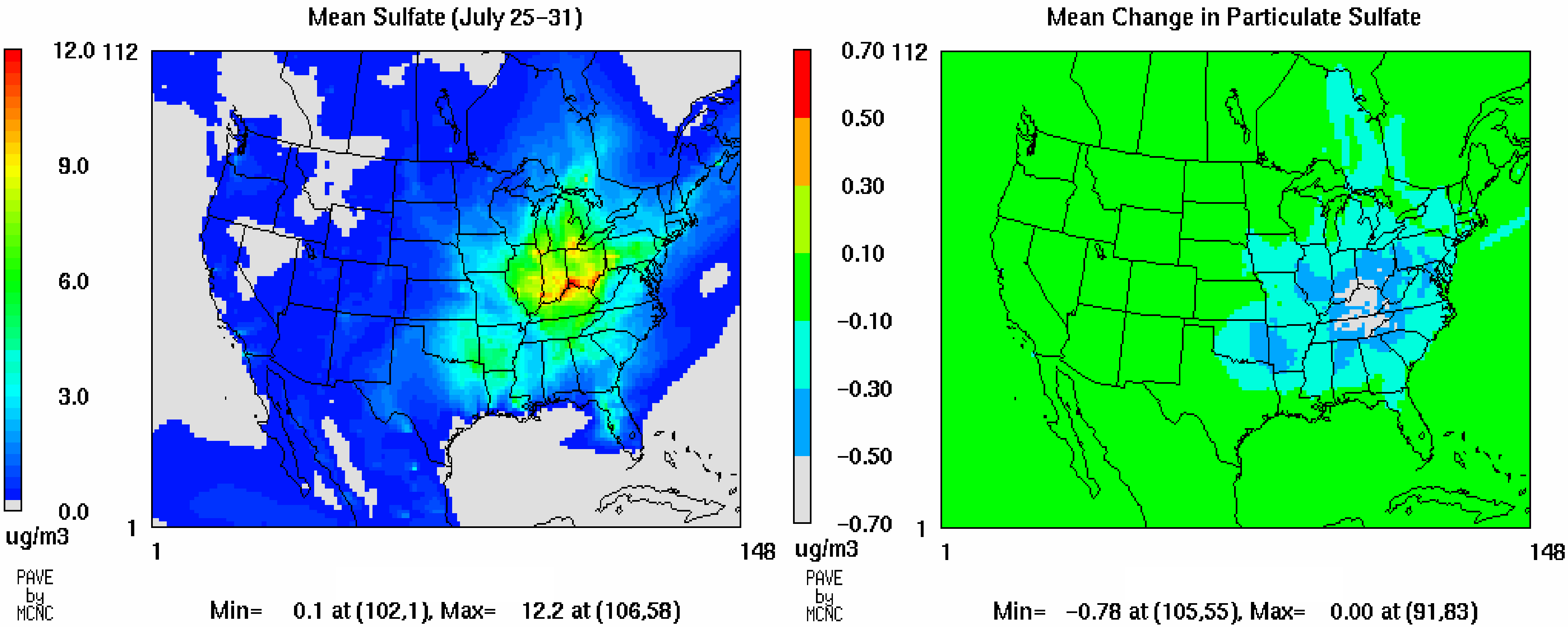
Giorgi (1986)

$$St = \frac{V_g u_*^{\,2}}{g\nu}$$

Effect of change in E_{im} on V_d for aerosols



Effects of change in aerosol V_d on SO_4 concentration

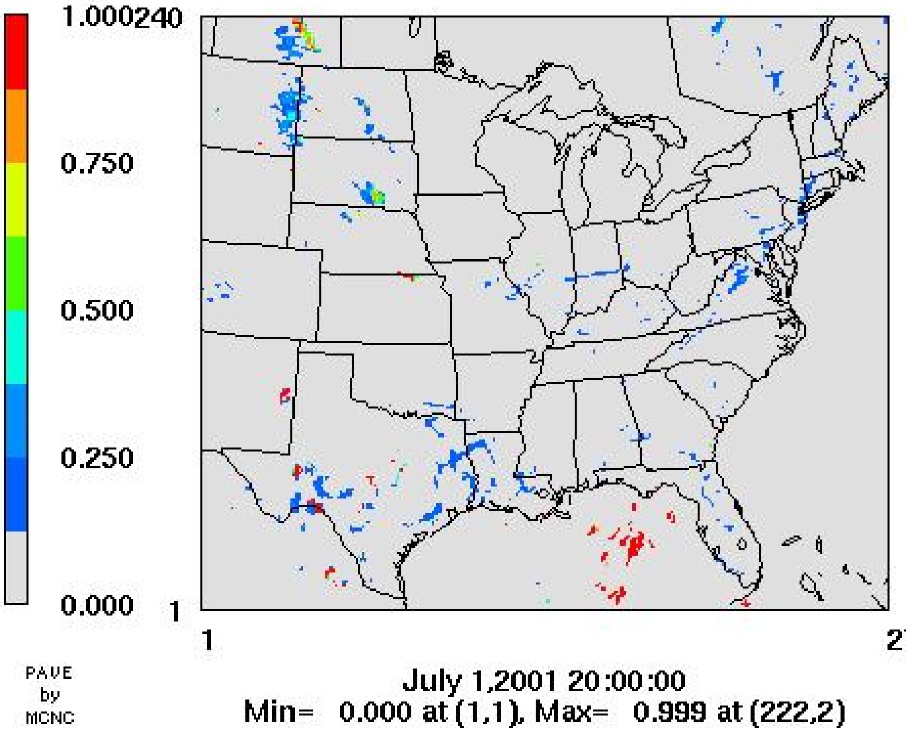


Modified convective cloud scheme

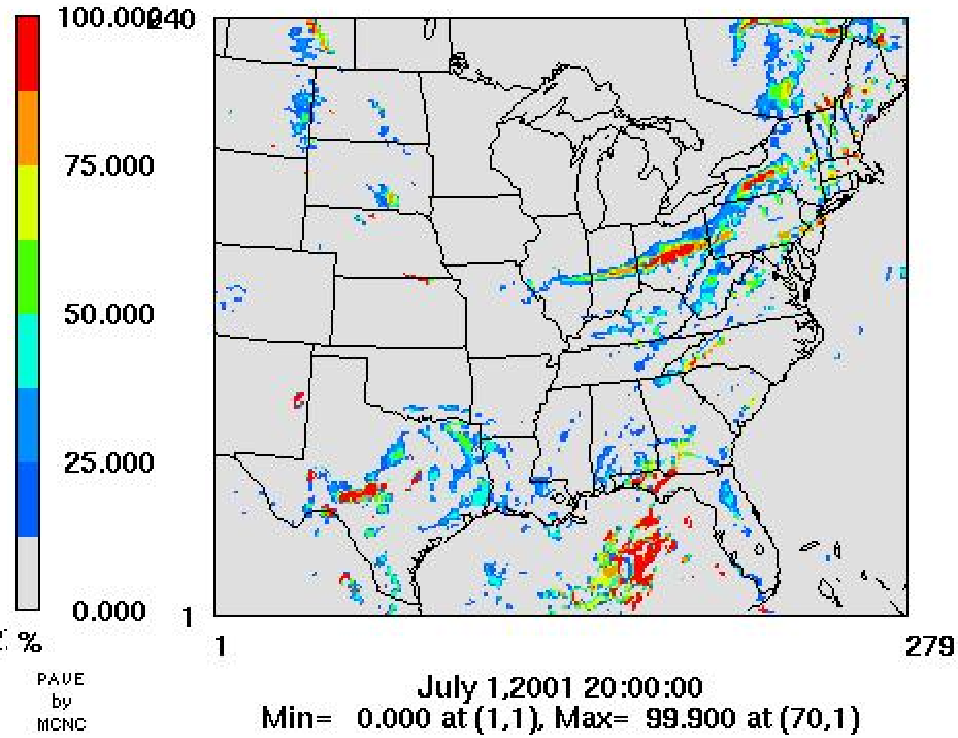
- Problems w/ convective scheme
  1. Excessive transport from upper layers to ground
  2. Artificial limitation of precipitating cloud coverage
- Solutions
  - Turned off cloud top entrainment
    - Reduces downward transport of high ozone concentration near tropopause
  - Replaced vertical mixing algorithm with ACM
    - Iterative mass limited time stepping eliminates artificial fractional area limitation
    - More gradual layer-by-layer compensating subsidence further reduces downward transport of upper layer air

Effects of cloud modifications on fractional area of precipitating clouds

RADM cloud model

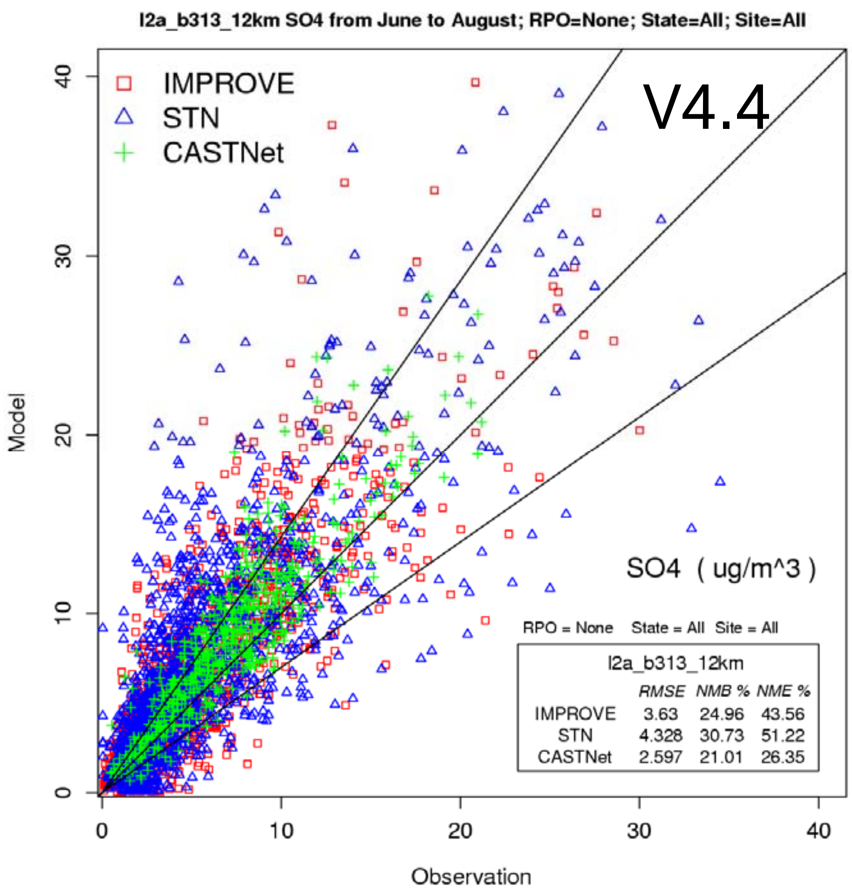


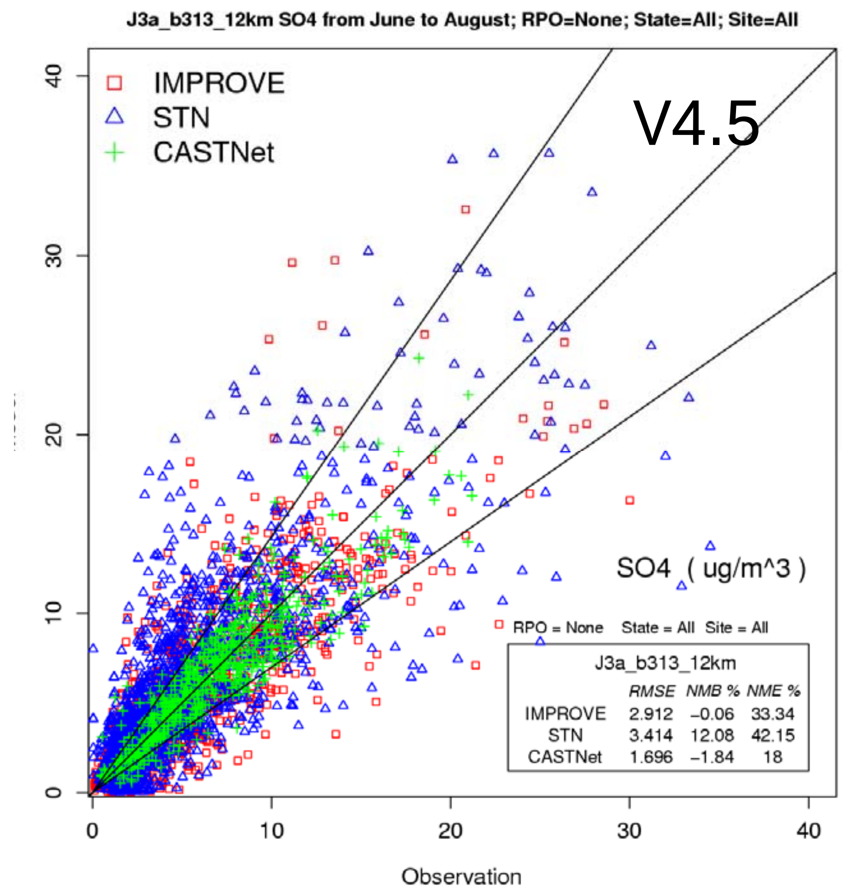
ACM-cloud model



What does it all mean?

12 km SO_4 for Summer 2001





Wyatt Appel will show more evaluation results

Coming down the pike

- CB05 Mechanism (Golam Sarwar's talk) – Beta release in October
- Mercury version – Interim release: 2006
- New in-line photolysis model for CMAQ (Frank Binkowski's talk)
- New PBL scheme for MM5, WRF, and CMAQ – ACM2

To Do List

- Develop a new convective cloud model that replicates meteorological convective schemes
  - collaboration w/ Georg Grell
- Implement operational satellite assimilation for
  - Surface insolation
  - Photolysis rates
  - Skin temperature nudging for soil moisture
  - Collaboration w/ UAH (Dick McNider)
- Develop on-line coupling capability for WRF-CMAQ through two-way coupler
  - Allow aerosol feedback to radiation model
  - Closer temporal coupling between meteorology and chemistry
  - Integrated resolved scale microphysics and aqueous chemistry

Disclaimer: The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number DW13921548. This work constitutes a contribution to the NOAA Air Quality Program. Althought it has been reviwed by EPA and NOAA and approved for publication, it does not necessarily reflect their views or policies.

Cloud processes in CMAQ

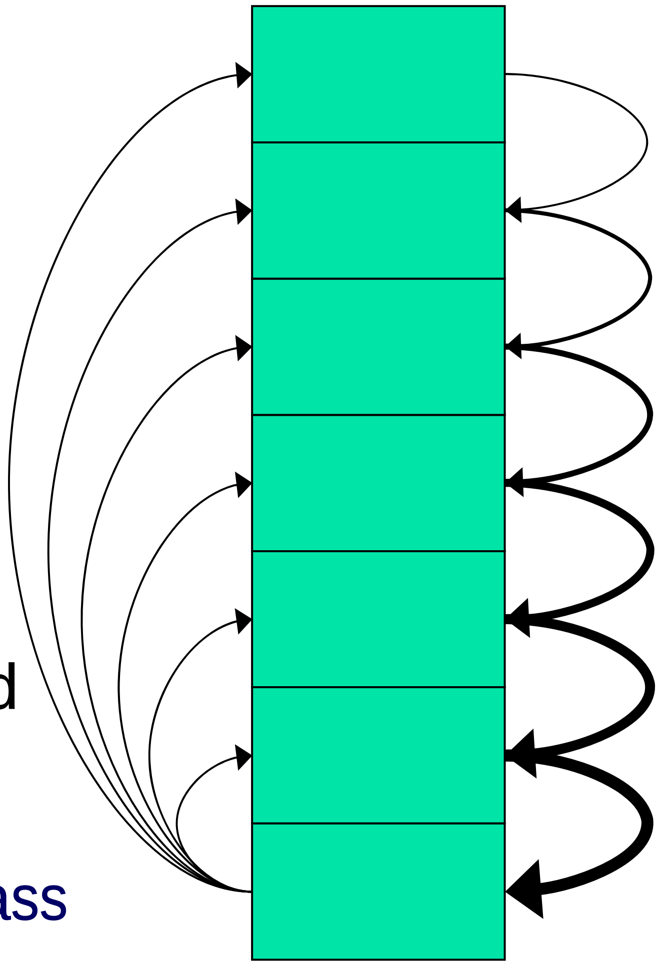
- Grid-resolved aqueous chemistry
  - Based on meteorology model output q_c, q_r
  - Wet deposition based on R_{nc}
- Subgrid convective clouds (RADM Cloud)
  - 1 hour cloudy box diagnosed by moist convective parcel
  - Detraining plume with side and top entrainment
  - Mixing closure by W_c/W_{ad} (Warner profile)
  - Precipitating cloud fraction based on R_c
  - Non-precipitating constrained by height and RH

ACM non-local mixing scheme was developed for PBL

$$M(z) = \frac{(1 - F(z))Frac}{3600}$$

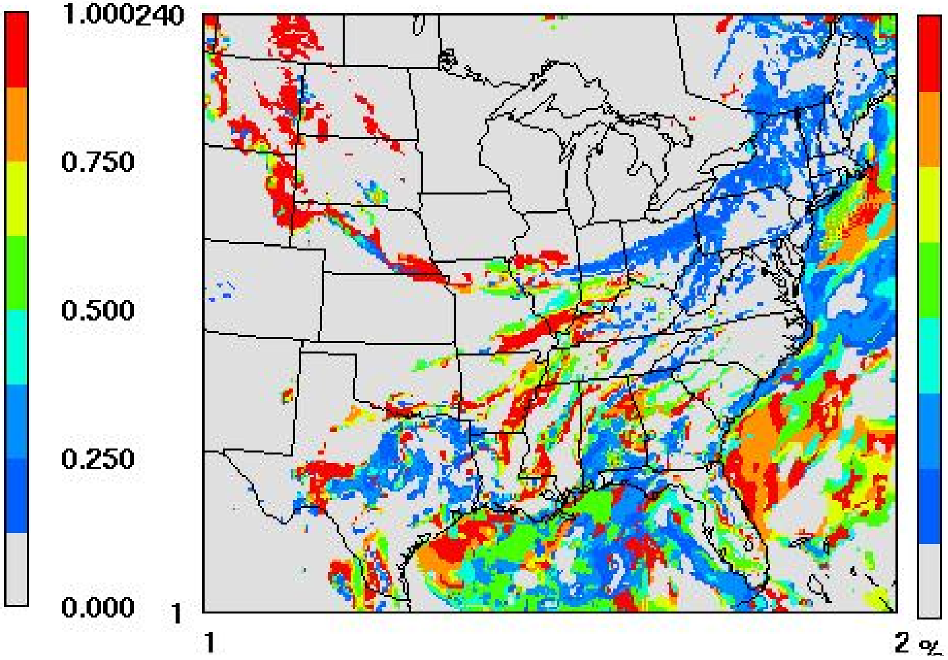
where *Frac* is the cloudy fraction of the grid column and *F(z)* is the cloud entrainment fraction.

Next step – use convective cloud mass flux scheme similar to met models (Buoyancy sorting)

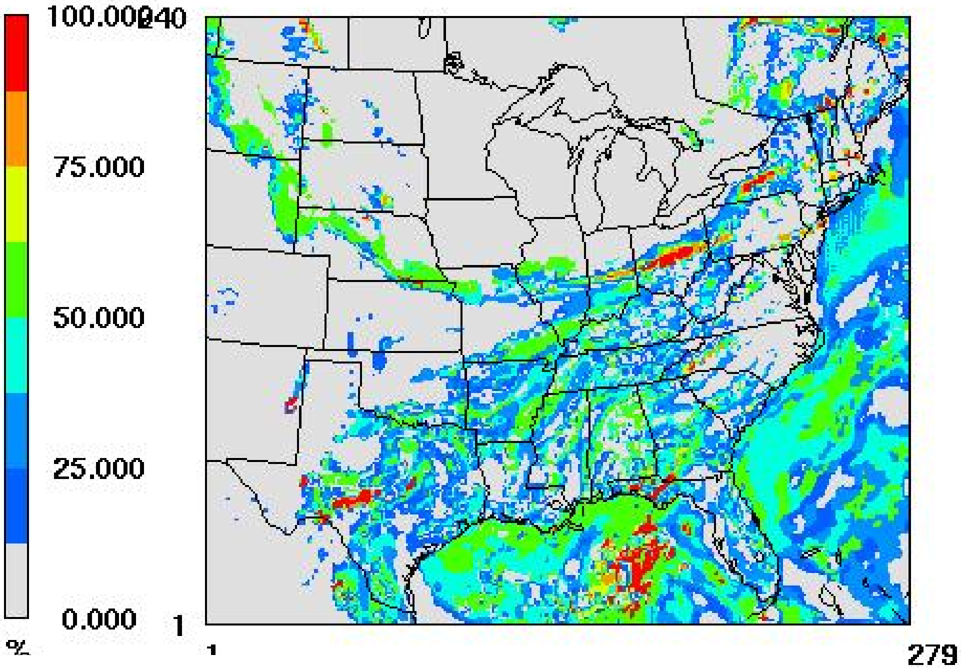


Effects of cloud modifications on fractional area of total convective clouds

RADM cloud model



ACM-cloud model



Precipitating + non-precipitating