Transport Processes in CMAQ

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Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

Outline

- Advection schemes
- Mass continuity
- Vertical diffusion
- Horizontal diffusion

Advection Schemes

Current model options:

- Peicewise Parabolic Method (PPM) (Colella and Woodward, 1984)
 - Monotonic scheme with geometric non-linear adjustments to the parabolic concentration distributions
- Bott (1989)
 - Forth order polynomial with positive definite flux limiter. A version with monotonic flux limiter has potential mass conservation problems

New schemes

- Total Value Diminishing (TVD) (Harten, 1983)
 - Piecewise linear with flux limiting for montinicity
 - Initial tests at Sandia: About 5 times faster than PPM with much less numerical diffusion.
- Walcek (2000)
 - Peicewise linear with monotone limiters and flux adjustments at local extremes. Well preserves low resolved peaks

Mass Continuity

- MM5/CMAQ is a non-hydrostatic, compressable, off-line model system
- Must correct advection results for inconsistencies in Mass and Momentum fields caused by:
 - Interpolations (time and space)
 - Inaccuracies in MM5
 - Numerical errors
- Current Release:

$$c_i J_s = \frac{\left(c_i J_s\right)^T}{\left(\rho_a J_s\right)^T} \left(\rho_a J_s\right)^{Int}$$

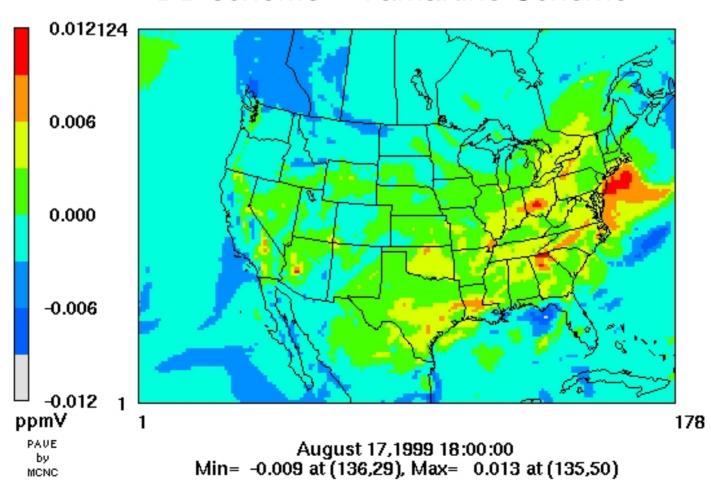
New advection corrections

- New scheme from Bob Yamartino
 - Solve mass continuity equation for vertical velocity for every vertical advection step
 - Correction for X,Y operator splitting
 - Already implimented in AQF system
- New time stepping scheme (CMAQ03)
 - Operator splitting time step set to Courant limitation for horizontal advection in lower layers
 - Upper layers allowed to take multiple advection steps per synchronization time step
 - User specified layers for synch step (default: σ =0.7)

Comparison of mass continuity schemas

Layer 1 Ozone

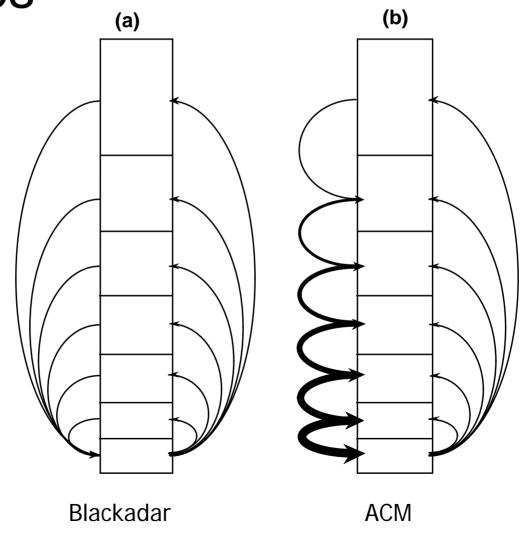
DB scheme – Yamartino Scheme



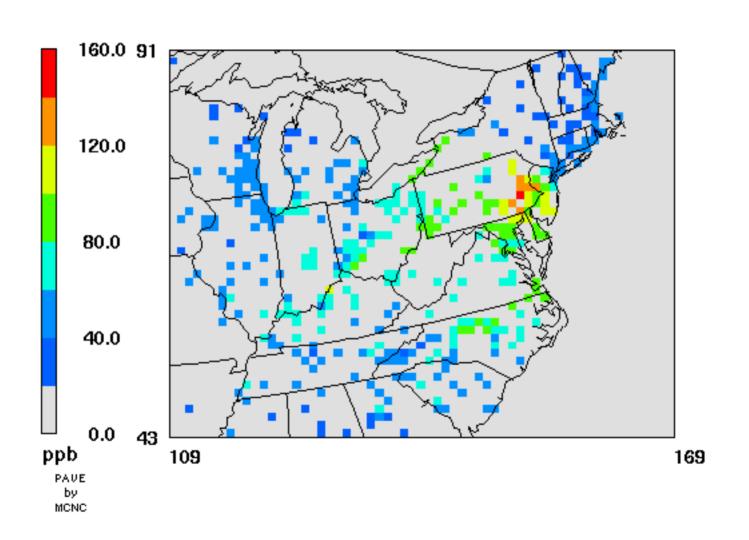
Vertical Diffusion

- Eddy Diffusion
 - Surface Layer and PBL scaling
 - Length scales: Z, h
 - Velocity scales: U*, W*
 - Layer integrated K_z
- Asymmetric Convective Model
 - Non-local convective scheme
 - Sensible heat closure
 - New local K₇ scheme when non-convective
- TKE (AQF System)
 - K_h from TKE model in Eta

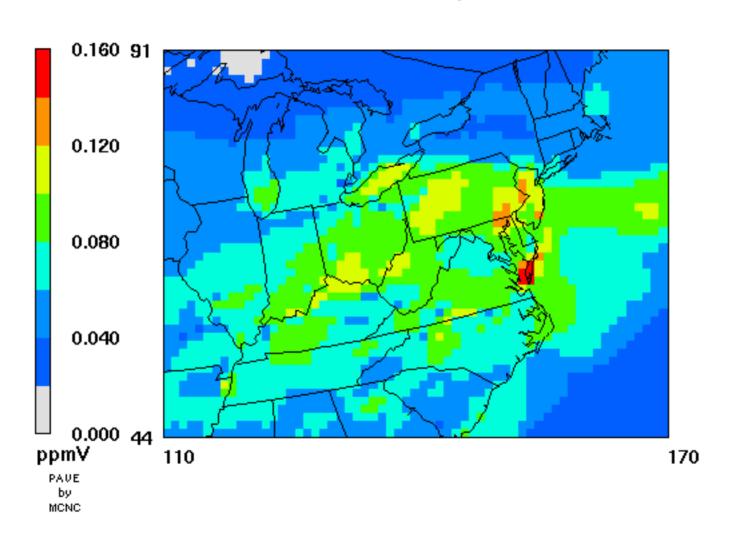
Convective Boundary Layer Schemes



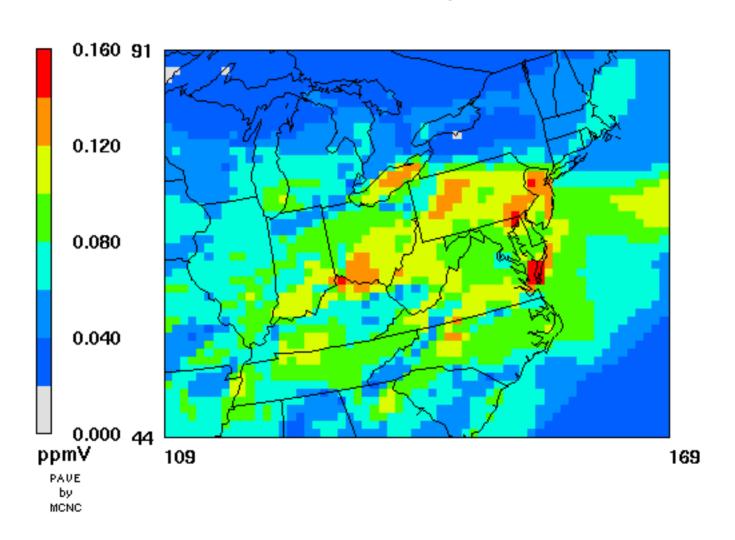
AIRS Ozone Obs, July 9, 1999, 21Z



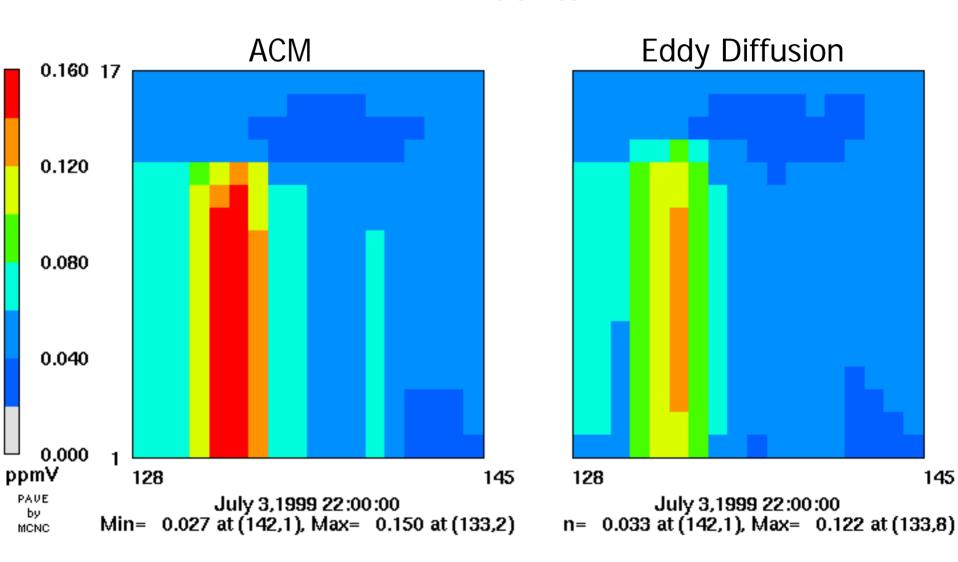
Base Model Ozone, July 9, 1999, 21Z



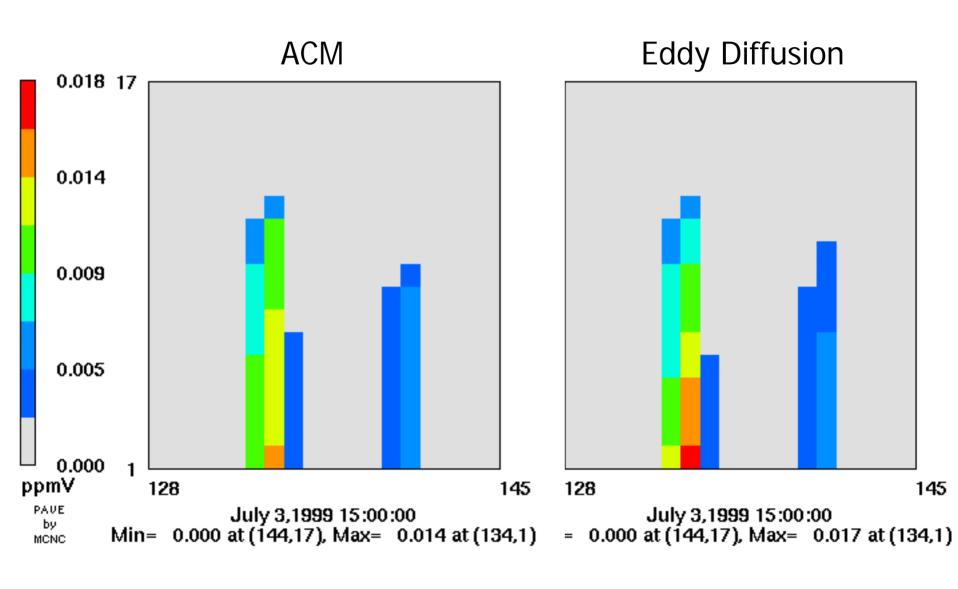
ACM Model Ozone, July 9, 1999, 21Z



Vertical cross-sections of ozone through Atlanta



Vertical cross-sections of NO_x



Next steps in Vertical Diffusion

- Updated Eddy diffusion (vertically continuous)
 - $K_z = ku_*/\phi_h(z/L)$ Zfunc
 - □ Zfunc = Z

- where Z < 0.1h
- □ ZFunc = $Z (1-Z/h)^2 1/(0.9^2)$ where Z > 0.1h
- New combined local & non-local scheme
 - Add local diffusion to ACM
 - Vertically continuous integration
 - Smooth transition from stable to convective
 - Need fast matrix solver

Horizontal Diffusion

- Current release:
 - Combined grid scale dependent background diffusivity and deformation dependent diffusivity following Smagorinski (1963)

$$K_{H} = \frac{K_{HA}K_{HD}}{K_{HA} + K_{HD}}$$

$$K_{HA} = K_{H_o} \frac{(\Delta x_{ref})^2}{(\Delta x)^2}$$

$$K_{HD} = \alpha^2 |D| (\Delta x)^2$$

$$D = \left[\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 \right]^{\frac{1}{2}}$$

$$K_{Ho} = 2000 \text{ m}^2/\text{s}$$

 $\Delta X_{ref} = 4000 \text{ m}$
 $\alpha = 0.28$

Next steps in Horizontal Diffusion

- Follow the SAQM work by Bob Yamartino
 - Account for numerical diffusion in advection scheme
 - Apply turbulence parameterization for physical horizontal diffusion
 - Account for horizontal wind shear