Mass Consistency Improvements in CMAQ Advection

Jeffrey Young, Jonathan Pleim and Rohit Mathur

Atmospheric Modeling and Analysis Division, National Exposure Research Laboratory, U.S. EPA, Research Triangle Park, North Carolina

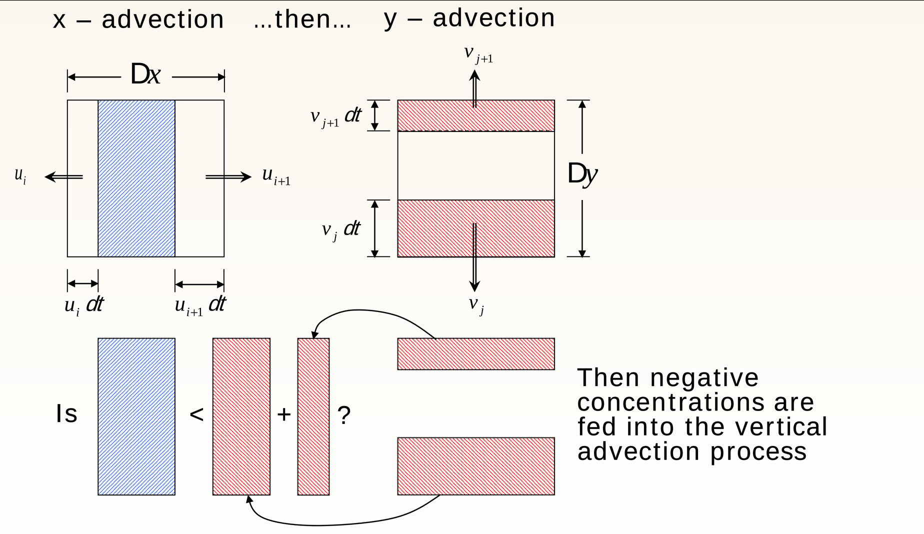
New Layer-Adjusted Advection Steps Determination

The operator-splitting paradigm used in CMAQ may cause intermediate negative concentrations to be generated for highly divergent wind fields in the horizontal advection process. Theoretically, these negative concentrations would then subsequently be resolved in the vertical advection algorithm. Situations have occurred where a solution cannot be found and the model terminates abnormally. The negative concentrations occur because the horizontal advection extracts more mass than is available in a grid cell (see Figure 1). This is caused by using an advection step that is too large.

CMAQ determines the advection time step based on satisfying the Courant-Friedrichs-Lewy (CFL) stability criterion. However the CFL-condition safe advection step does not consider the issue posed by wind fields with high divergence regions.

One possible solution is to globally set a smaller value for the maximum allowable synchronization step. However, this approach results in much longer run times, in effect being penalized by a relatively small number of occurrences of high divergence in the wind fields.

A new method has been developed in which the advection time steps calculation has been modified to include satisfying a horizontal divergence criterion as well as the CFL condition.



Required: $hdiv = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \approx \frac{u_{i+1} - u_i}{\Delta x} + \frac{v_{j+1} - v_j}{\Delta y}$; δt ' $hdiv\ \delta t < 1$

Figure 1. Schematic of Horizontal Advection

Advection/Synchronization Step Algorithm

1. Set ATOP
   - Synchronization step = advection step at least up to this level
   - From environment variable or default sigma level = 0.7
2. Find max **U / Δx** in lower layers up to ATOP and determine a trial, max advection step. **δt** that satisfies an adjusted Courant-Friedrichs-Lewy condition (***ACFL***): **Uδt / Δx** < 0.75
3. Set the synchronization step = **δt** for each layer up to ATOP
   - Keep the synchronization step between 60 and 720 sec
   - If the synchronization step should be < 60 sec in order to satisfy the ***ACFL***, set it to 60 and adjust **δt** to satisfy the ***ACFL*** and evenly divide the synchronization step
4. For layers above ATOP, the same synchronization step is used, but **δt** could be decreased to satisfy the ***ACFL***
   - In each layer above ATOP, find max **U / Δx** and if necessary, adjust **δt** to satisfy the ***ACFL*** and evenly divide the synchronization step
5. For all the layers, find the maximum horizontal divergence, ***hdiv*** and adjust **δt** if ***hdiv*** **δt** > 1 by halving **δt**

Steps 1-4 were in the previous version; step 5 is new.

The modeled transport of pollutant species is sensitive to the advection time step, therefore differences are observed comparing the new method with globally setting a small advection time step. Figure 2 shows 24 hour runs for 5 Aug 2006 in a 153x171x34, 4 km Houston, TX domain of the new algorithm vs. an imposed 100 sec. maximum synchronization/advection time step. The latter took <u>twice</u> as long to run.

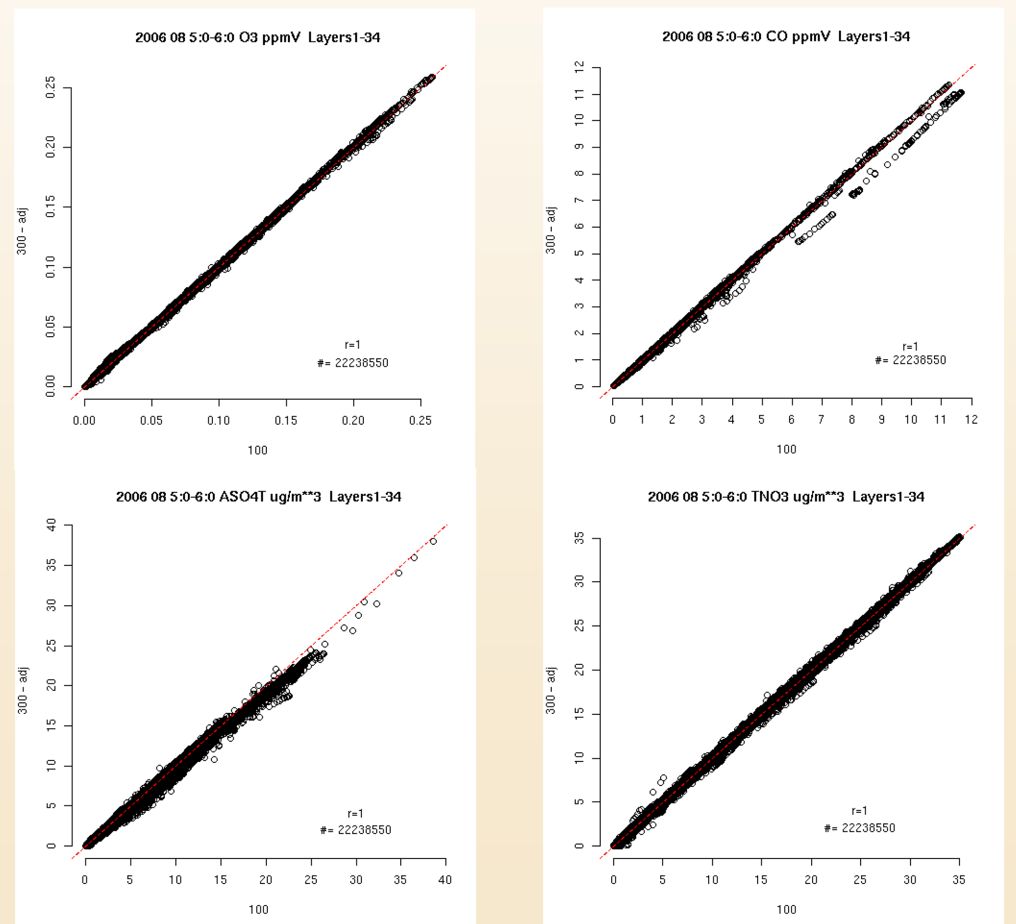


Figure 2. Comparing the New Algorithm vs. the Standard Method

New Mass-Consistent Vertical Advection

The mass-conserving advection scheme in CMAQ uses an upwind donor cell method for the vertical component, which is known to be first order numerically diffusive. We have implemented a higher-order, less diffusive scheme that adjusts the diagnosed mass fluxes using the Piecewise Parabolic Method (PPM).

In the current version (informally called "yamo," after Bob Yamartino) the rediagnosed vertical velocities, v_i are calculated using:

$$f_i = (\rho_M - \rho_T)\Delta\sigma/\delta t + f_{i-1};\ \ v_{i+1} = f_i/\rho_T;\ \ v_1 = 0;\ f_0 = 0$$

Where, in the i_{th} layer, ρ_M is the met density, ρ_T is the transported density, $\Delta\sigma$ is the vertical grid cell spacing, and δt is the time step.

Using these velocities, the concentrations, including ρ_T are vertically advected. If necessary, the vertical velocities are adjusted to keep the CFL < 1, and the concentrations are recalculated.

In the new version (informally called "yamop"). the velocity is further adjusted by the ratio of the upwind fluxes (f_U) to the PPM calculated fluxes (f_P). This step is repeated, if necessary, until the differences between f_U and f_P are less than a small tolerance. Then the concentrations are advected using PPM with the final recalculated vertical velocities.

Comparison of the rediagnosed vertical velocities with the WRF velocities in Figure 3. shows good agreement up to the top layer. The excess or deficit mass is adjusted up through the layers with the topmost serving as a kind of reservoir.

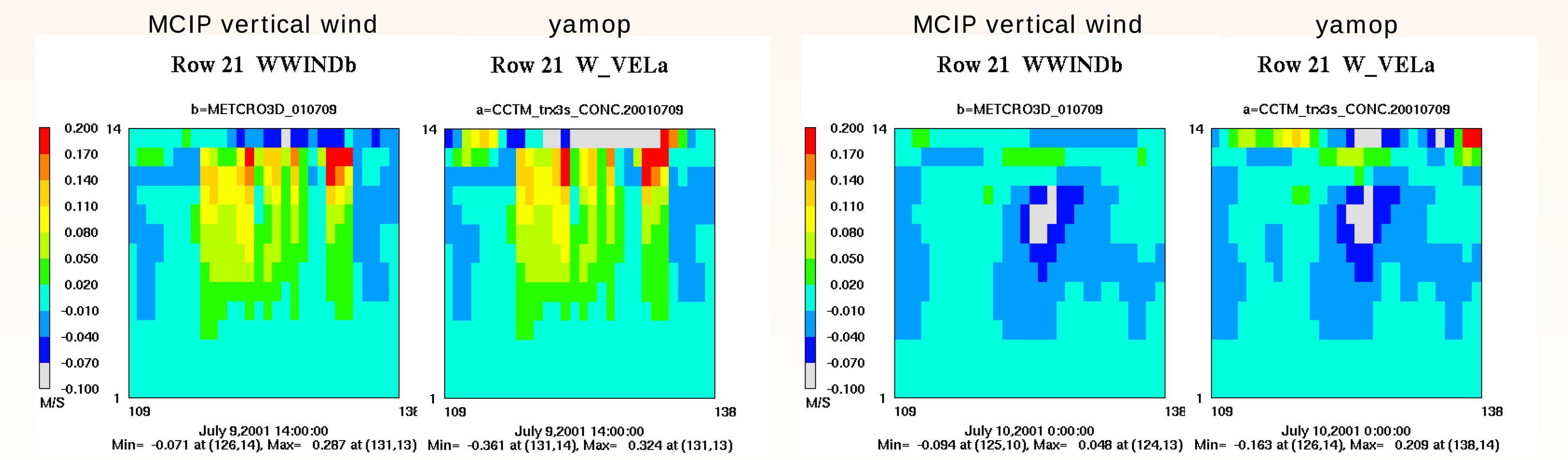


Figure 3. Vertical Velocities thru Lower FL for 36 Km, 148x112x14, July 2001 Selected Hours

The more numerically diffusive nature of the standard "yamo" compared with the new "yamop" can be seen in Figures 4 and 5, where the cross section in Figure 5 is the same as in Figure 3.

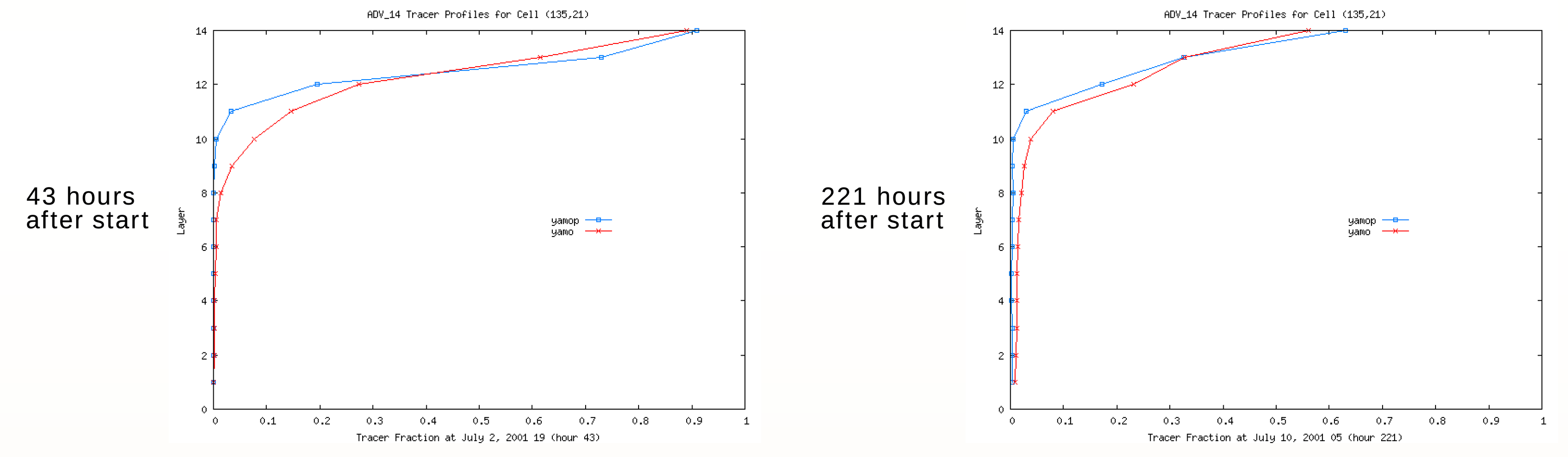


Figure 4. Vertical Profiles of Advection-Only Tracer Species Initialized to 1 in the Top – 36 Km, 148x112x14, July 1-14, 2001, Grid Cell 135,21

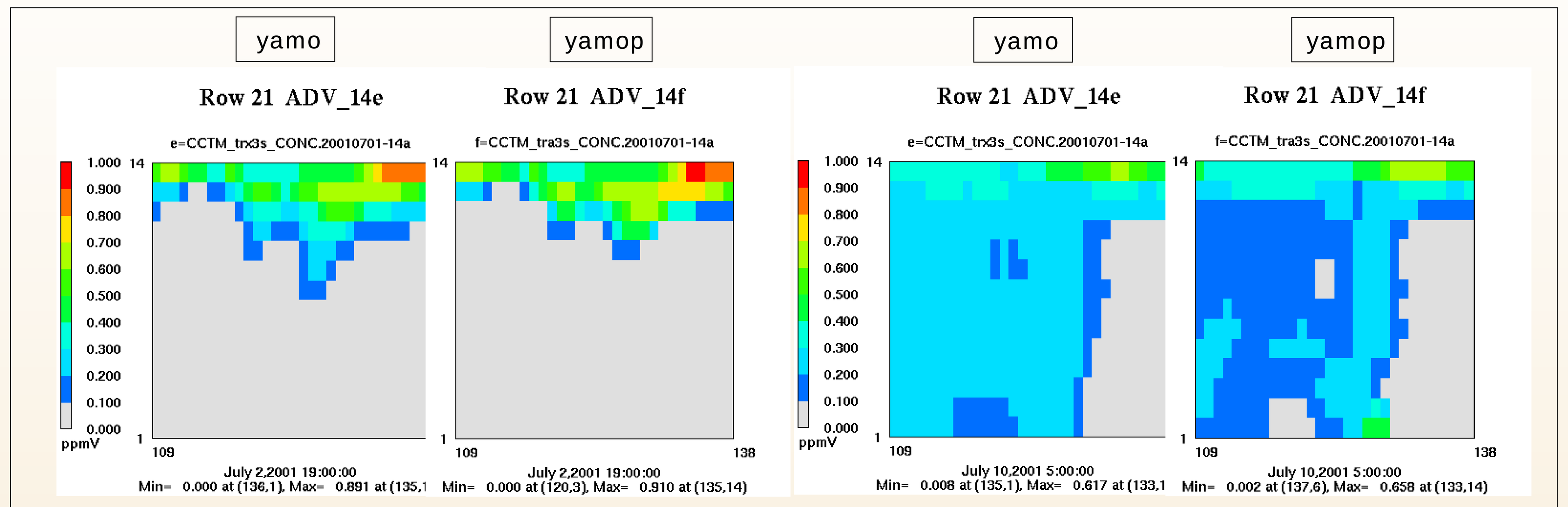


Figure 5. Profiles of Advection-Only Tracers thru Lower FL for Two July 2001 Selected Hours

These results have a significant effect on surface level concentrations, and consequently also on dry deposition, e.g. as seen in Figure 6.

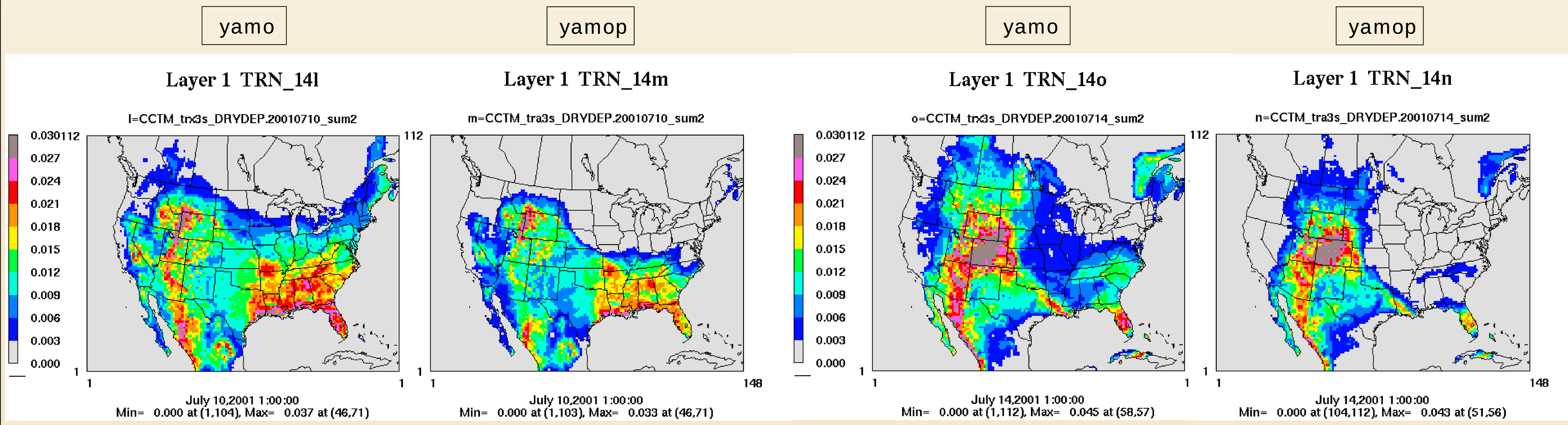


Figure 6. 24 Hour Accumulated Dry Deposition of Transport Tracer Species Initialized to 1.0 in the Top Layer – No emissions, Chemistry or Aerosol Processes on July 10 and July 14, 2001

Layer Collapsing Issues

In order to reduce computational time and output data sizes in CMAQ, a technique can be used in MCIP which takes generated 34 layer meteorology fields, for example and reduces them to "equivalent" 14 layer fields for use in CMAQ, thereby reducing CPU time and other computer resources. To a certain extent, this procedure destroys consistency between the meteorology variables, and for applications such as the long-range transport of pollutants, it is not recommended. Figure 7 shows a comparison of the layer structure for a typical collapsing from 34 to 14.

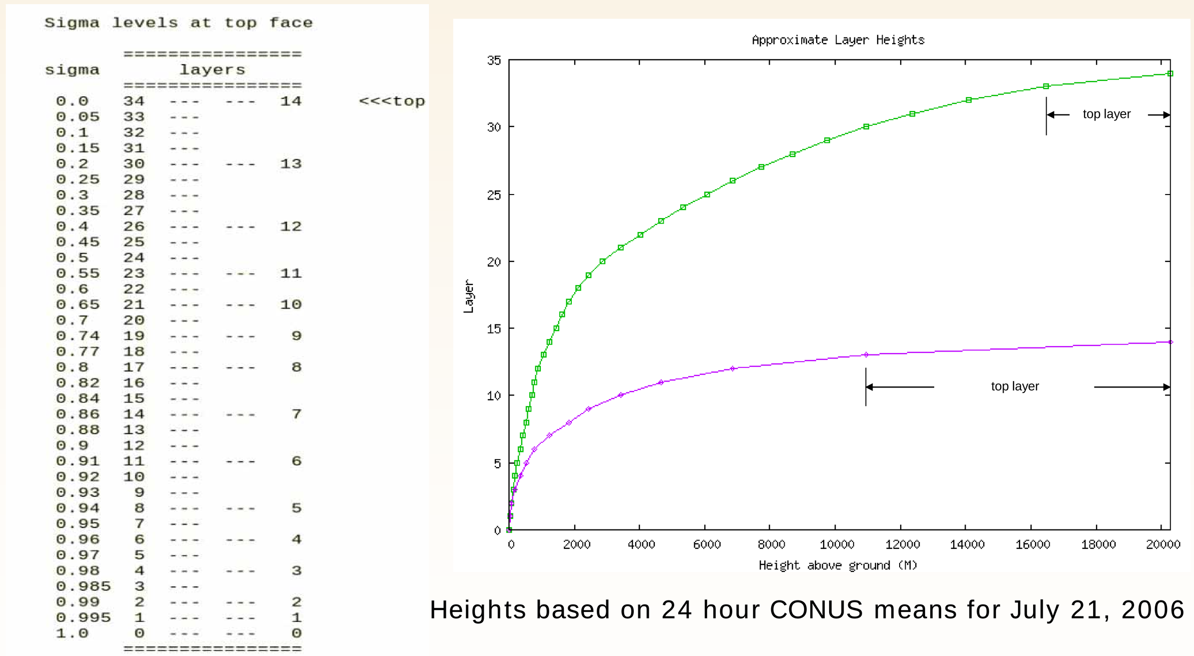


Figure 7. 14 Layers vs. 34 Layers

As in the previous section ("New Mass-Consistent Vertical Advection"), experiments were run with two types of tracers:

- Tracer species for mass transport (TRN)
  transport = advection + diffusion + dry dep + clouds + wet dep
  (The dry deposition velocity was set to the value for O3)
- Tracer species for advection only (ADV)

These tracer species were initialized to 1.0 only in the top layers, including the boundary concentrations. The initial concentrations were set to zero elsewhere. For example, TRN_34 was set to 1.0 in layer 34 and 0.0 elsewhere, TRN_33 was set to 1.0 in layer 33, etc. These were all run with the new "yamop." The meteorology used was a 34 layer July 21-26, 2006 USGS 12 Km CONUS and 14 layer collapsing in MCIP.

Figures 8 and 9 describe some results of concentrations and dry deposition with tracers initialized in the top layers. As can be seen, a significant amount of mass has migrated from the top to layer one in the 14 layer run as compared to the 34 layer run.

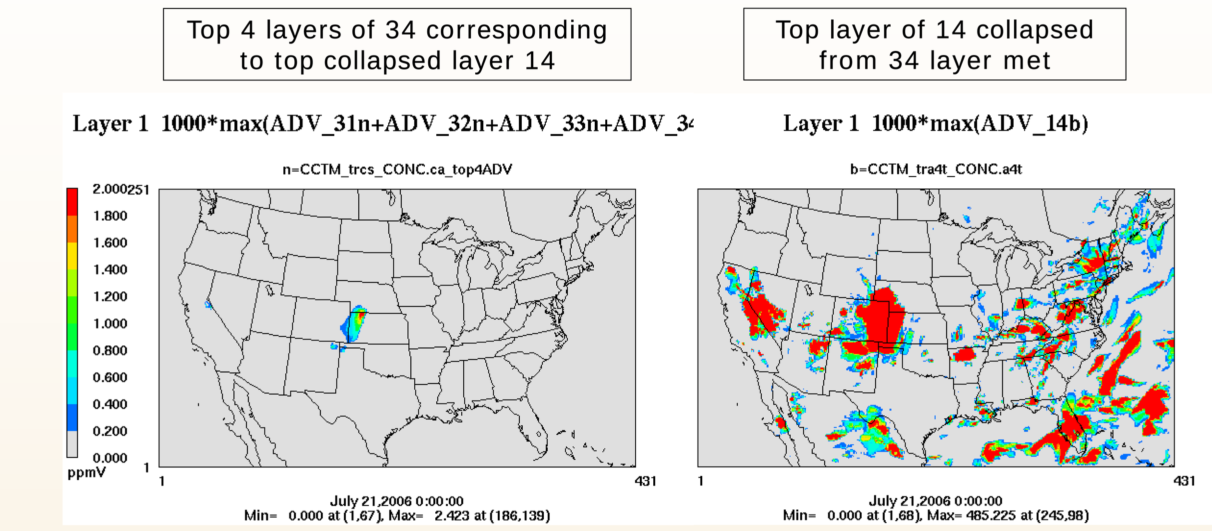


Figure 8. Layer One Comparison of Top Layer(s), Advection-Only Tracers Concentrations (24 Hour Max)

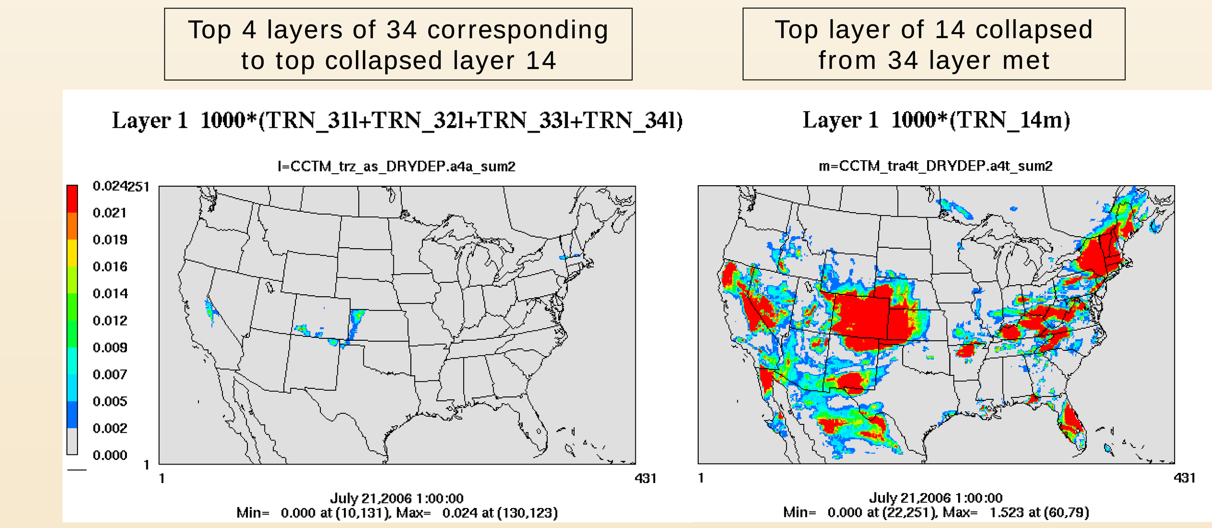


Figure 9. Comparison of 24 Hour Dry Deposition Accumulation of Top Layers Transport Species