AN IMPLEMENTATION OF THE TRAJECTORY-GRID ADVECTION ALGORITHM IN CMAQ

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1. INTRODUCTION

Numerical diffusion is a serious problem for the Eulerian advection algorithms typically used in chemical transport simulators for air quality modeling. This extra diffusion damps local extremes and smears steep gradients in trace species concentrations, for example, those due to localized emissions of primary pollutants such as NOx and VOC's. This, in turn, compromises the model's chemistry calculations of the production of secondary pollutants, such as ozone, which depend nonlinearly on the relative concentrations of the precursors. In order to remove this source of inaccuracy, a Lagrangian advection algorithm called Trajectory-Grid (TG) has been implemented in the EPA's Community Multiscale Air Quality (CMAQ v4.4) model. The TG algorithm for advection follows representative air "packets" along trajectories determined by the wind field. The air composition in a packet is unchanged by advection. The resulting prototype simulation model is called CMAQ-TG. The TG algorithm was introduced by Chock et al. (1996, 2005) and a version has been implemented in CAMx.

CMAQ-TG uses the same meteorology, emissions, initial conditions, boundary conditions, and photolytic rates input as standard CMAQ, making "apples-to-apples" comparison of standard CMAQ and CMAQ-TG possible. Our comparison shows that CMAQ-TG advection produces a non-diffusive solution and maintains linearity of the advection and diffusion processes.

In this discussion, "standard" CMAQ means CMAQ v4.4 with

- PPM (Piecewise Parabolic Method) used for horizontal and vertical advection
- Eddy diffusion (K-theory) used for horizontal and vertical diffusion
- CB4 or SAPRC99 gas chemistry with the associated EBI solver

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2. IMPLEMENTATION OF CMAQ-TG

In this section, we give a brief description of the key features of our incorporation of the TG approach into CMAQ code.

The primary modification made to standard CMAQ was to replace the separate horizontal advection (HADV) and vertical advection (VADV) modules with a single 3-D Lagrangian advection module called ADVEC_TG. Because the TG approach transports packets, each with a set of mixing ratios, it conserves mass as long as the input meteorology data are mass consistent, see Chock et al. (2005). Therefore, there is no need to invoke a mass correction routine. Also, CMAQ-TG does not use Couple & Decouple to convert between mixing ratios and concentrations, but instead maintains gas phase composition solely in the form of mixing ratios. The present prototype version of CMAQ-TG supports advection, diffusion, gas chemistry, emissions, and dry deposition.

2.1 Role of an Eulerian Grid in CMAQ-TG

Input to CMAQ, such as meteorological data, emissions data, initial conditions, and boundary conditions, is all associated with the cells of an Eulerian grid on the model domain. Also, output from CMAQ is most easily saved as gridded data using **netCDF**, and viewed using **PAVE**. For these two reasons alone, it is necessary to easily relate packet position to grid cell indices. Furthermore, some processes that are potentially global in nature, such as eddy diffusion, do not have satisfactory Lagrangian models at this time and are therefore modeled on the Eulerian grid. Finally, grouping packets in the same grid cell together is a convenient way to keep track of which packets are close to each other. Thus, the primary data structure for listing packets in CMAQ-TG is an array of lists of the packets in each grid cell, indexed by the column, row, and layer indices of the CMAQ Eulerian grid. The main data used to characterize each packet are simply the (x, y, z) coordinates of its location in the model domain and an array of mixing ratios for the species of interest.

Although an Eulerian grid is necessary in the current CMAQ-TG environment, whenever possible, it plays no role once input data have been assigned to initial packet locations. For example, this is the case for the advection, dry deposition, emissions, and gas chemistry processes.

2.2 External Sources and Sinks

Emissions are converted to changes in mixing ratios based on cell volume. Once this has been done, the same change in mixing ratios is applied to each packet in a cell. Dry deposition is calculated packet-by-packet. In CMAQ-TG, these processes have been broken out from vertical diffusion as independent subroutines, allowing greater flexibility in managing the sequence in which the CTM science processes are performed. Source and sink processes are performed at the start of each synchronization time step, before the transport processes of advection and diffusion.

2.3 Advection

Lagrangian algorithms come in many different flavors. The TG approach to advection uses packets distributed throughout the simulation domain at roughly the same resolution as the underlying grid. Thus there are at most a few packets in each grid cell, as illustrated by Fig. 1. This differs from many other Lagrangian algorithms where a high density distribution of particles has been used to support the goal of simulating sub-grid scale dispersion.

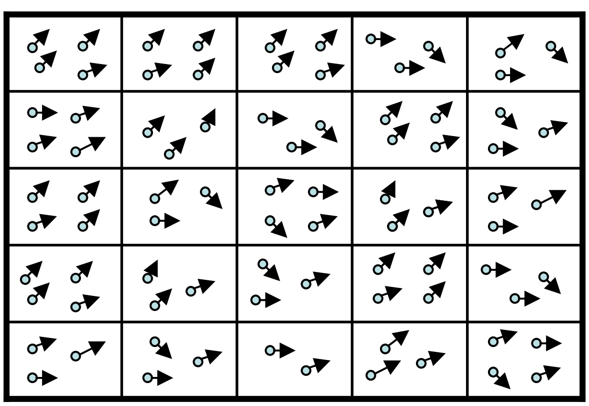

Fig. 1. Packets in the cells of a horizontal layer of a CMAQ-TG domain.

The packets are small volumes of air, carrying the mixing ratios of the chemical species of interest, which move along trajectories determined by the wind field.

2.4 Packet Management

Packet management is done to balance the density of packets in cells between the competing goals of covering the solution domain - to ensure completeness and accuracy - and limiting computational expense. The packet management tasks of “spawning”, to create new packets in cells with too few packets, and “pruning”, to remove packets from cells that are overpopulated, are done as part of the advection process.

Although packet management has strong benefits, it has some negative aspects as well.

- Spawning requires initializing new packet composition using some type of interpolation which is likely to be somewhat inaccurate and diffusive.
- Aggressive spawning, e.g., never allowing a cell to be empty, may be unnecessary if a nearby packet will soon move into the cell.
- Pruning can throw away good composition information which could be used later in the simulation if the need for spawning a replacement is discovered.

2.5 Diffusion

The underlying algorithms for both vertical and horizontal diffusion are very close to those in standard CMAQ, see Byun and Ching (1999) for details. The discussion here focuses on the changes made to accommodate packets.

The requirements we set for the CMAQ-TG diffusion algorithms are:

1. For each species and cell, the average of the packet mixing ratios after a diffusion step should be the same as the cell mixing ratio obtained from Eulerian diffusion of the previous averages.
2. For each species, the maximum and minimum packet mixing ratios after a diffusion step should be within the range of values at the beginning of the step; in particular, this ensures that positive mixing ratios remain positive and that the maximum does not increase.
3. Linearity.

Initially we thought that horizontal and vertical diffusion could be adequately handled by doing Eulerian diffusion of cell averages and then adding cell deltas to the individual packets in cells.

However, testing showed that this fast and simple procedure fails to satisfy our second requirement. Then, an initial method we tried for fixing this problem failed to satisfy the third requirement, linearity. These problems have now been fixed, see Table 1.

The horizontal diffusion process includes a sub-grid diffusion step to account for diffusion between packets in the same cell that is very similar to what is described in Chock et al. (2005). As was noted in that paper, further investigation of this algorithm is clearly needed.

Table 1. Linearity tests of the transport algorithms (advection and diffusion) with a realistic wind field. Linearity for CMAQ-TG is excellent.

	IC1_BC1 - IC1_BC0 - IC0_BC1	
	CMAQ-TG	**Standard CMAQ**
Layer 1	(-0.0000, 0.0000)	(-0.0190, 0.0238)
Layer 13	(-0.0000, 0.0000)	(-0.2316, 0.1127)
Row 31	(-0.0000, 0.0000)	(-0.0867, 0.0468)

	SPOS_A - SPOS_B - SPOS_C	
	CMAQ-TG	**Standard CMAQ**
Layer 1	(-0.0005, 0.0015)	(-0.3704, 0.3227)
Layer 13	(-0.0010, 0.0013)	(-2.0829, 1.4139)
Row 31	(-0.0028, 0.0021)	(-0.2743, 0.2470)

2.6 Chemistry and Other Processes

Chemistry in CMAQ-TG is processed for packet mixing ratios instead of grid cell mixing ratios. Otherwise, it is unchanged from standard CMAQ. In the future, support for all CMAQ processes, including aerosols and cloud/aqueous phase, will be added.

2.7 Output

Several representations of cell composition are available, each in its own file, including:

- **AVG_MIX**: species-wise average mixing ratios over the packets in the cell
- **CLS_MIX**: mixing ratios for the packet horizontally closest to the cell center
- **MAX_MIX**: species-wise maximum mixing ratios over the packets in the cell
- **MIN_MIX**: species-wise minimum mixing ratios over the packets in the cell
- **OLD_MIX**: mixing ratios for the oldest packet in the cell

The **PACKET** file contains the following information for each cell

- **COUNT**: Number of packets
- **NEW_PACKETS**: Number of new packets added during output step
- **AVG_AGE**: Average age of the packets
- **MAX_AGE**: Age of the oldest packet

At this time, output is limited to grid cell quantities and we depend on **PAVE** to view results.

3. EVALUATION WITH IDEALIZED 2-D WIND

In this section, we evaluate the horizontal transport processes for properties such as preservation of peak values. First we look at advection alone, and then at advection with horizontal diffusion.

3.1 Advection with 2-D Rotation

The wind field used in this section is a steady, two-dimensional rotation through 360^o every 24 hours.

One of the critical shortcomings of Eulerian advection algorithms is numerical diffusion. As demonstrated by Fig. 2, a high frequency 2Δx signal, the checkerboard pattern, is quickly lost when advection is simulated using the Eulerian piecewise parabolic method (PPM) in standard CMAQ.

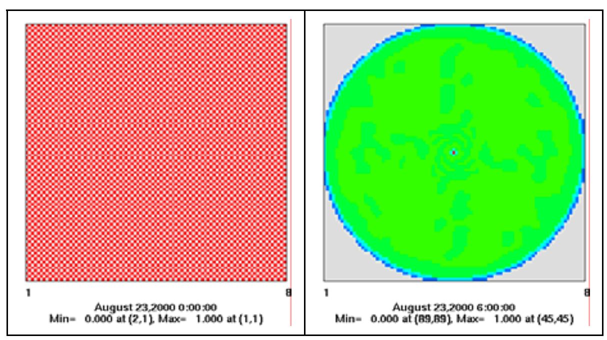

Fig. 2 Loss of high frequency signal due to the numerical diffusion of the PPM scheme.

In contrast, Fig. 3 shows the behavior of CMAQ-TG in an example where all cell have been initialized with 4 evenly spaced packets and the AVG_MIX display is used. We see that CMAQ-TG preserves the checkerboard pattern almost perfectly after 6 hours, during which the packets go through a 90^o rotation.

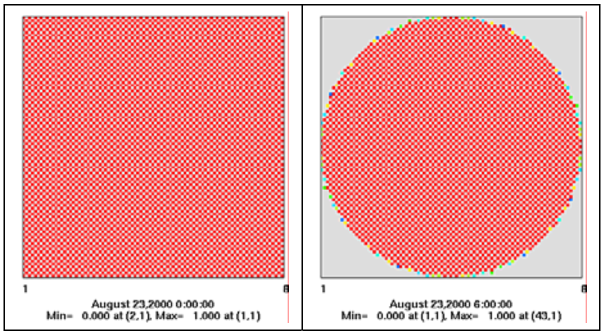

Fig. 3 CMAQ-TG preserves the checkerboard pattern almost perfectly after 6 hours.

In a second example, we compare CMAQ-TG with standard CMAQ using advection of a mound of a peak height of 50. The initial profile for both simulations is shown in Fig. 4.

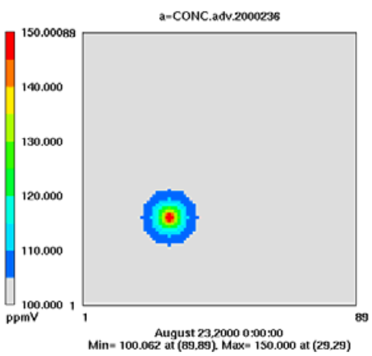

Fig. 4 Initial profile of a mound to be advected by the circular wind field.

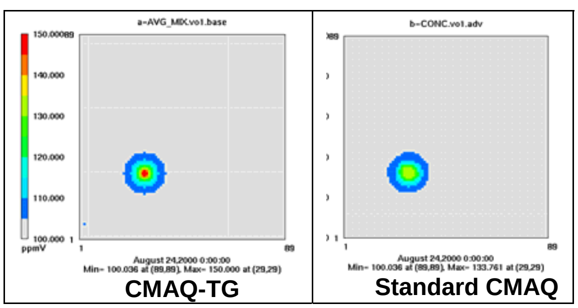

Fig. 5 After 24 hours, CMAQ-TG has preserved the peak height while standard CMAQ has reduced it by over 30%.

Fig. 5 shows the results from the two versions of CMAQ after 24 hours – one full rotation. The comparison shows that TG advection preserves amplitude, while the numerical diffusion of PPM advection significantly dampens the peak of the mound, bringing it down by over 16 ppm from the initial height of 50 ppm above the background value.

3.2 Advection plus Horizontal Diffusion with 2-D Rotation

The result of repeating the comparison shown in Fig. 5 with horizontal diffusion added to the simulation is shown in Fig. 6. The magnitude of the difference here is significantly smaller that in Fig. 5. This suggests that as more processes are incorporated, the effect of using different advection algorithms, Lagrangian or Eulerian, becomes less apparent.

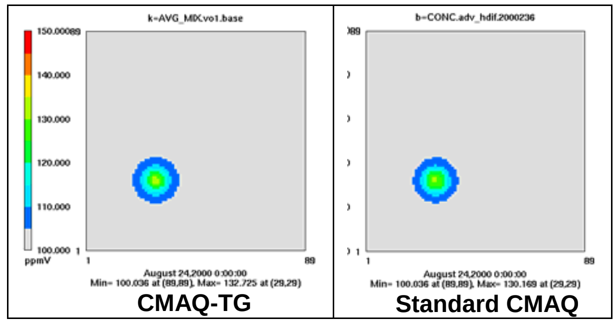

Fig. 6 The same as Fig. 5, but showing the difference between CMAQ-TG and standard CMAQ for advection with horizontal diffusion.

4. EVALUATION WITH REALISTIC 3-D WIND

Although a two-dimensional rotational field provides an interesting controlled opportunity to study transport characteristics, we must also test with realistic meteorology. In particular we now use 3-D output from MM5 for August 25, 2000.

4.1 Comparison of 3-D Advection and Transport

Fig. 7 compares transport of the checkerboard and IC1_BC0 (initial conditions = 1, boundary conditions = 0) patterns by the TG and PPM advection algorithms after 24-hours. The results show that 3-D movement of the checkerboard pattern by PPM and TG produce qualitatively similar results. However, the PPM results show a smoothed concentration field, resulting from numerical diffusion, while the graininess of the TG results indicates that the checkerboard pattern is being preserved.

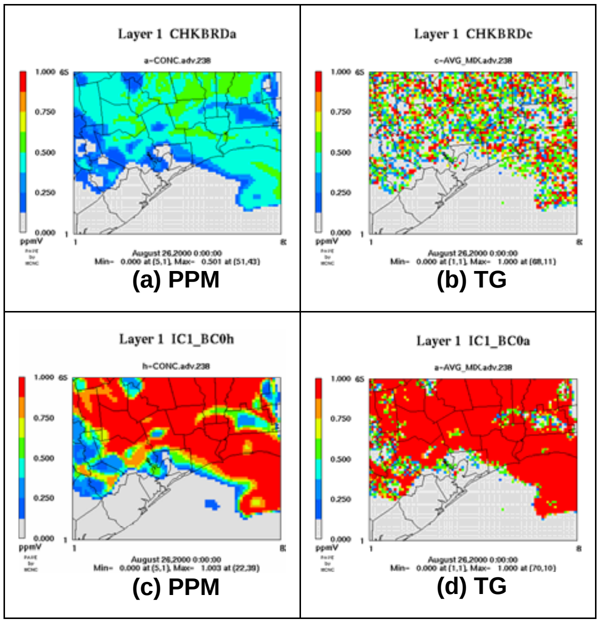

Fig. 7 Advection of the checkerboard and IC1_BC0 signals by a three-dimensional wind field from MM5 after 24 hours. The signals are affected by the transport of packets from the upper layers.

Fig. 8 shows a vertical cross section of the vertical velocity field from MM5 and a snapshot of the number of packets being used in TG. It shows that packets are moved by the updrafts and downdrafts and therefore the signals are affected by the transport from upper layers.

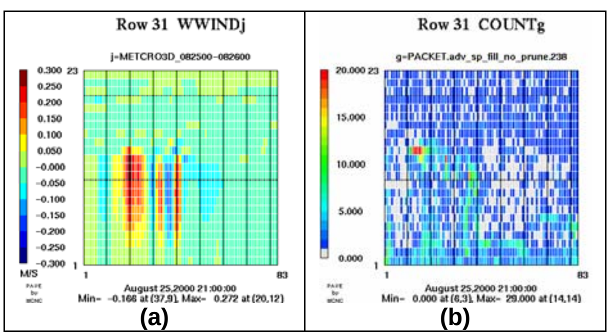

Fig. 8 (a) Vertical cross section of the vertical velocity field across row 31, and (b) number of packets used in the TG calculation with a three-dimensional wind field from MM5.

When the horizontal and vertical diffusion processes are added to advection, the difference between standard CMAQ and CMAQ-TG transport is significantly reduced as in Fig. 9

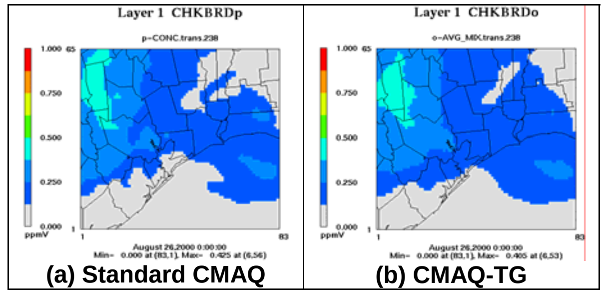

Fig. 9 Results of TG advection with horizontal and vertical diffusion of the checkerboard pattern after 24 hours.

4.2 Preliminary Testing of CMAQ-TG for Ozone Simulation

The next step in the CMAQ-TG code verification process was to study the interaction of the transport modules with the gas-phase chemistry module. Because of the high nonlinearity of the chemistry module, and due to the non-diffusive nature of Lagrangian advection, we expected CMAQ-TG to exhibit a somewhat wider range of chemical concentrations than standard CMAQ. The simulation in this section includes CB4 gas phase chemistry, emissions, dry deposition, advection, and diffusion.

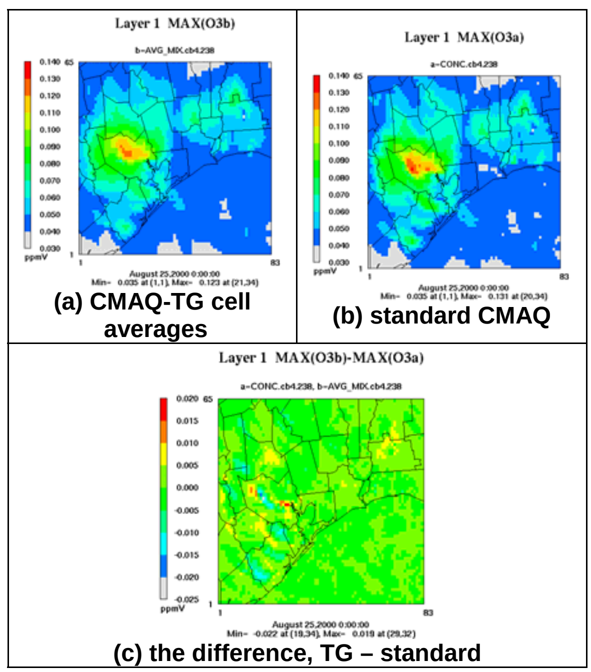

Fig. 10 Comparison of daily maximum ozone values simulated by CMAQ-TG and standard CMAQ.

In Fig. 10 we compare daily maximum ozone values simulated by CMAQ-TG and standard CMAQ. Note that, while standard CMAQ yields the highest daily maximum ozone value, by 8 ppb, CMAQ-TG produces individual cell values that differ from standard CMAQ by as much as -22 ppb below and 19 ppb above. CMAQ-TG shows the largest difference above standard CMAQ near the Houston Ship Channel, a site with high emissions.

5. CONCLUDING REMARKS AND FUTURE DIRECTIONS

In its current form, CMAQ-TG supports many of the basic physical processes required for a CTM, including advection, diffusion, gas chemistry, emissions and dry deposition. The TG technique eliminates the serious spurious diffusion associated with Eulerian methods, without introducing other side effects such as false oscillations and negative concentrations. However, another form of numerical diffusion may be introduced by the packet spawning process that is part of the current packet management strategies. Basic versions of packet management tasks have been implemented, but effective packet management may be the biggest obstacle to CMAQ-TG becoming competitive with standard CMAQ. Several useful representations of cell composition are available. But, displaying results using existing tools designed for uniform grid structures causes information loss, so improved display methods are needed.

6. ACKNOWLEDGMENT AND DISCLAIMER

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