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**Trajectory Grid Transport Algorithm
in CMAQ**

Final Report

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Atmospheric and
Environmental Research, Inc.

Final

Trajectory Grid Transport Algorithm in CMAQ

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Submitted to

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EXECUTIVE SUMMARY

Under CRC Project A-55, the Trajectory Grid (TG) advection algorithm was implemented within the Community Multiscale Air Quality Model (CMAQ) (Byun and Percell, 2006). This prototype version is hereafter referred to as CMAQ-TG-UH. (CMAQ-TG will be used to refer to a version with improved mixing ratio conservation characteristics [see below].) TG advection uses a Lagrangian approach and follows individual “packets” of concentrations as each traverses in the grid system following a three-dimensional wind trajectory. The objectives of this project are to (1) provide an independent evaluation of the prototype of CMAQ-TG-UH, (2) describe how TG may be used to reduce advective transport errors and (3) if applicable, make improvements to the implementation in CMAQ to reduce artificial diffusion and provide a better understanding of the turbulent diffusion process.

A South Coast Air Basin test case from July 2005 was used based on consultation with Dr. David Chock, Ford Motor Company, and Dr. Satoru Mitsutomi, South Coast Air Quality Management District.

In a simple test case without emission, due to a post-diffusion mass adjustment step carried over from CMAQ, CMAQ-TG-UH did not conserve mixing ratio of a tracer with constant initial and boundary mixing ratios as well as expected (1-3% error). This step was unnecessary for CMAQ-TG-UH, which was formulated based on mixing ratios. Removal of this post-diffusion mass adjustment significantly improved the conservation of mixing ratios (0.001% error). The implementation without mass adjustment is hereafter referred to as CMAQ-TG and is used for further analysis in this project.

For the South Coast Air Basin test case, when CMAQ-TG was applied with physical diffusion deactivated, TG was confirmed to be inherently less diffusive in both horizontal and vertical directions than the grid-based advection scheme of CMAQ. An emission-diffusion simulation showed that CMAQ and CMAQ-TG shared similar diffusion results. Therefore, the diffusion behavior of CMAQ-TG was controlled by the treatment of inhomogeneous concentration packets within each grid cell by the diffusion scheme. Several tests were performed on the diffusion algorithm. The UH algorithm for packet diffusion included a likely double counting of subgrid diffusion. The first test

involved removing the explicit subgrid diffusion step, but resulted in only a small change in the diffusion behavior. A second test involves the implementation of a purely grid-based diffusion step followed by a subgrid diffusion step, similar to the implementation of Chock et al. (2005). Mixing ratio gradients were significantly sharper in this simulation. Therefore, we concluded that the UH diffusion algorithm was more diffusive than the original Chock et al. (2005) algorithm. Because of the confounding effects among physical diffusion, artificial diffusion, and grid cell dilution in a traditional Eulerian air quality model, the diffusion module has seldom undergone rigorous independent investigation. How best to model turbulent diffusion is an open science question, with possible approaches including parameterized diffusion (such as the algorithms used in this project) or a Lagrangian particle dispersion model. The TG advection scheme provides an opportunity to support future investigations into the behavior of diffusion schemes without confounding numerical effects.

The predictions of CMAQ-TG, especially pertaining to vertical transport, were sensitive to packet management strategies. Upper level predictions, typically represented by fewer packets than near surface, can benefit from a strategy that can avoid excessive pruning and subsequent spawning of new packets. However, the effects of the packet management strategy varied with time and did not appear to be systematic on the dispersion characteristics of the mixing ratio field of an inert tracer.

TABLE OF CONTENTS

1. INTRODUCTION	1
2. TEST CASE.....	3
3. EVALUATION OF CMAQ-TG-UH.....	4
3.1 Examination of Computer Code	4
3.2 Behavior of CMAQ and CMAQ-TG-UH in a Simple Test Case	7
3.3 Evaluation of Packet Management	10
4. EVALUATION OF TRANSPORT WITHIN CMAQ-TG.....	14
5. ALTERNATIVE PACKET MANAGEMENT	24
6. CONCLUSIONS.....	26
7. ACKNOWLEDGMENTS	27
8. REFERENCES	28

LIST OF FIGURES

Figure 3-1 Schematic of CMAQ-TG-UH and CMAQ	5
Figure 3-2 CO mixing ratio (16-hour average) for CMAQ with transport only.....	8
Figure 3-3 CO mixing ratio (16-hour average) for CMAQ-TG-UH simulations with transport only with and without mass adjustment	11
Figure 4-1 CO mixing ratio at hour 8 (16 GMT) for CMAQ and CMAQ-TG simulations with advection and emission only.....	15
Figure 4-2 CO mixing ratio at hour 8 (16 GMT) for CMAQ and CMAQ-TG (UH diffusion scheme) simulations with diffusion and emission only.....	17
Figure 4-3 CO mixing ratio at hour 8 (16 GMT) for CMAQ-TG with transport and emission only, using the implementation of horizontal and vertical diffusion by UH	19
Figure 4-4 CO mixing ratio at hour 8 (16 GMT) for CMAQ-TG with transport and emission only, using the implementation of diffusion by UH for grid diffusion only.....	21
Figure 4-5. CO mixing ratio at hour 8 (16 GMT) for CMAQ-TG with transport and emission only, using an implementation of diffusion similar to Chock et al. (2005)	22
Figure 4-6. CO mixing ratio at hour 8 (16 GMT) for CMAQ-TG with transport and emission only, using an alternative diffusion treatment based on the UH implementation	23
Figure 5-1. CO mixing ratio at hour 8 (16 GMT) for CMAQ-TG with transport and emission only, using an alternative packet management strategy without pruning	25

LIST OF TABLES

Table 3-1 Packet management in the South Coast Air Basin test case.....	11
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1. INTRODUCTION

Eulerian air quality models embody the state-of-the-science knowledge in atmospheric transport and chemistry using a fixed reference frame. Model formulation or structural uncertainties are unavoidable because gaps exist in the current understanding of atmospheric processes and because simplifications are typically used in the mathematical representation of complex systems. Parametric uncertainties arise from inaccuracies in either input data or parameters. Even when model and parametric uncertainties can be minimized, the numerical solutions to the differential equations that represent advection, diffusion, vertical mixing, deposition, and chemical processes are subject to uncertainties.

Due to the use of the operator splitting approach, air quality models are typically designed to be modular. For a given time step, modules of advection, diffusion, chemistry, and other processes, are called consecutively, where the spatial and temporal changes of concentrations due to one process are solved while other processes are ignored. This approach allows the development of optimal methods to solve a particular kind of differential equation. Traditionally, numerical methods for solving the advection equation on a discretized spatial grid system have been a subject of active research, because of the need to reduce numerical diffusion associated with the solution. The advection equation is:

$$\frac{\partial C}{\partial t} + \frac{\partial(uC)}{\partial x} + \frac{\partial(vC)}{\partial y} + \frac{\partial(wC)}{\partial z} = 0 \quad (1)$$

where the concentration is a function of time (t) and space (x, y, z), and u, v, and w are the wind components in the x, y, and z directions, respectively. Note that TG is actually designed to solve the general concentration form of Equation (1). To avoid having to deal with spurious mass adjustment or similar steps in some air quality models, and in view of the generally small mass conservation errors inherent in some flow fields, it is applied to the mixing ratio format, such that C has units of ppm (Chock et al., 2005). In this case the velocity in Equation (1) is also taken out of the partial derivatives. The advection equation can be written in other forms and coordinate systems. EPA's Community Multiscale Air Quality model (CMAQ) has offered a variety of schemes in various versions, including the Bott scheme (Bott, 1989), the piecewise parabolic method

(PPM; Collela and Woodward, 1984), and the Yamartino scheme (Yamartino, 1993). So far, none of these numerical schemes has been shown to be free of numerical diffusion.

Under CRC Project A-55, the Trajectory Grid (TG) advection algorithm was implemented within CMAQ (Byun and Percell, 2006). This prototype version is hereafter referred to as CMAQ-TG-UH. TG was originally developed by Chock et al. and implemented in the PMCAMx air quality model (Chock et al., 1996, 2005). The underlying concept of TG is to use a Lagrangian approach and follow individual “packets” of concentrations as each traverses in the grid system following a three-dimensional wind trajectory. During the advection process, the packets move based on the local wind conditions, but otherwise experience no change in mixing ratios. In this advection formulation, therefore, the concentrations in mass per volume (or mole per volume) change as densities change, and mixing ratios are conserved.

The objectives of this project are to (1) provide an independent evaluation of the prototype of CMAQ-TG-UH, (2) describe how TG may be used to reduce advective transport errors and (3) if applicable, make improvements to the implementation in CMAQ to reduce artificial diffusion and provide a better understanding of the turbulent diffusion process. In air quality models, a physical diffusion module is typically included to represent the turbulent diffusion, e.g., using the K theory. The term artificial diffusion is used here to refer to unintended diffusion, which can arise from several sources. A common source is the numerical diffusion associated with the advection scheme. For grid models, dilution of point concentrations into a grid cell volume can also cause artificial diffusion. In the case of a Lagrangian approach within an Eulerian framework, there are uncertainties in the model representation of the diffusion process, e.g., treatment of grid or subgrid diffusion. Due to model uncertainties, modeled diffusion can be less than or greater than true diffusion. At present, numerical diffusion and physical diffusion cannot be separated in models that treat both advection and diffusion. Because of its minimal likelihood in generating numerical diffusion in the advection step, TG can be very useful for studying true diffusion and its impact on air quality.

2. TEST CASE

Chock et al. (2005) used a test simulation from the Southern California Ozone Study (SCOS) in August 1997. Although this would have been an ideal test case for the present work, the meteorological input files for PMCAMx were not compatible with CMAQ. South Coast Air Quality Management District (SCAQMD) was approached to obtain the proper input files. Dr. Satoru Mitsutomi of SCAQMD advised against using the August episode because it was older and the performance was not satisfactory (personal communication, 6 March 2008). For evaluating advection algorithms implemented in CMAQ, Dr. Mitsutomi recommended the July 2005 episode. The July 2005 episode has been thoroughly characterized in the Air Quality Management Plan (AQMP; 2007). Dr. Chock also agreed on the desirability of Southern California as a test bed. For the AQMP, all 2005 episodes, including the July episode used here, were developed using the MM5/CAMx model combination. Therefore, we obtained CAMx emissions input files as well as MM5 output files for the July 2005 episode. CMAQ-ready meteorological files were prepared using the Meteorology-Chemistry Interface Processor (MCIP) version 3.3. The two-dimensional surface emission file for CAMx was converted to NetCDF format. An in-house processor was used to calculate plume rise for stationary sources based on the algorithm within SMOKE to generate a three-dimensional NetCDF format file for upper air emissions.

The prototype CMAQ-TG-UH was implemented in version 4.4 of CMAQ. Therefore, the stock version of CMAQ 4.4 was used as a bench mark in this study. The PPM scheme was used for horizontal and vertical advection in CMAQ. The Multiscale scheme was used for horizontal diffusion and Eddy diffusion was used for vertical diffusion.

3. EVALUATION OF CMAQ-TG-UH

3.1 Examination of Computer Code

A schematic of CMAQ-TG-UH, as it is currently implemented, is shown in Figure 3-1. This schematic contains transport and gas-phase chemistry (CHEM) routines. Aerosol and cloud processes are not shown because they are not implemented. The corresponding schematic for CMAQ is shown for comparison.

When implementing CMAQ-TG-UH, Byun and Percell separated out the surface processes originally solved in the vertical diffusion (VDIFF) routine, including dry deposition (DRYDEP) and emission (GETEMIS). These changes make the code more transparent and allow a user to diagnose the effects of various processes more easily.

For TG, advection in three dimensions is simulated concurrently and in mixing ratio (ppm) units (ADVEC_TG). After the advection procedure, the TG routine also checks for empty cells and creates new packets in a process called “spawning” or “filling,” where necessary. Every few time steps, excess packets are also deleted in a process called “pruning.” Through the use of an environment variable set in the run script to execute the model, the user can define how frequently pruning takes place.

The corresponding processes in CMAQ are more complicated. The horizontal (XADV and YADV) and vertical advection (ZADV) processes in CMAQ are formulated in conservation (flux) form, and the unit used for concentrations is “coupled” with the coordinate Jacobian and the local density. It may be easier to think of the coupling (COUPLE) and decoupling (DECOUPLE) processes as unit conversions from mixing ratio (used in vertical diffusion and chemistry) to a density-based concentration unit (amount per volume, used in advection and horizontal diffusion) and back to mixing ratio. In addition, there is an adjustment routine (ADJADV) that corrects for mass consistency error in the meteorological data. This module conserves mixing ratio, and is considered an integral unit of the physical advection process, together with the horizontal and vertical advection routines (Byun and Schere, 2006).

It should be noted that mass adjustment represents a fairly contentious issue within the air quality modeling community. In an ideal world, if the meteorological

CMAQ-TG-UH CMAQ

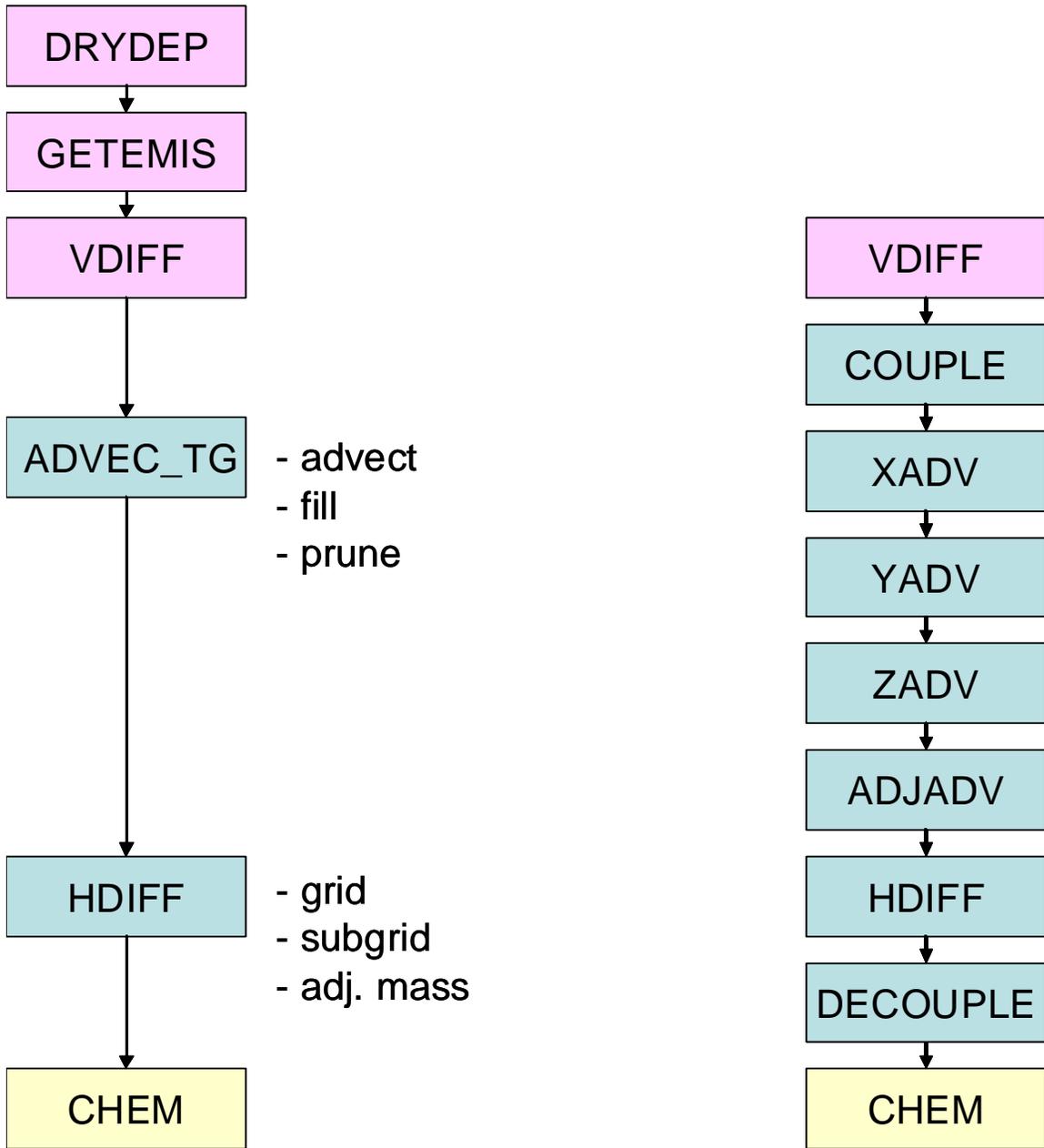


Figure 3-1. Schematic of CMAQ-TG-UH and CMAQ. See text for definition of routines.

model conserves mass properly and mass-conserving meteorological fields are provided to air quality models at sufficient time resolution, a mass conservation step need not be implemented in the air quality model. In CMAQ-TG-UH, the implicit assumption behind tracking mixing ratios is that the mass concentration prediction of CMAQ-TG will be subject to the mass conservation errors in the input meteorology fields. Chock et al. (2005) showed that such errors were not always substantial. Therefore, it is computationally more advantageous to use the mixing ratio form directly rather than the concentration form and at the same time obviate the use of arbitrary mass adjustment. On the other hand, the mass adjustment procedure within CMAQ adjusts concentrations of advected species to account for the difference between the advected density and the input density. If the advection scheme is numerically perfect, this step adjusts only the mass conservation errors introduced by the meteorological inputs. In reality, however, this step also corrects for any inaccuracies introduced by the advection scheme itself. Therefore, the adjustments can be somewhat arbitrary and can be propagated throughout the simulation. Because of the somewhat different and inconsistent assumptions used in the implementation of the mixing ratio based vs. flux based approaches, a side by side comparison may alternatively put CMAQ-TG at a disadvantage or be subject to criticism because the mass correction step is considered to be an integral part of the density-based advection formulation in CMAQ.

The horizontal diffusion process (HDIFF) is treated in mixing ratio units in CMAQ-TG-UH but in density-coupled units in CMAQ. The TG version accounts for grid-scale diffusion and subgrid-scale diffusion. As implemented by UH, the grid-scale diffusion step accounted for the interaction between individual packets within one grid cell and average concentrations of nearby cells. The subgrid scale diffusion step accounted for the interaction between individual packets with the average concentration within the same cell. This implementation was different from Chock et al. (2005), which accounted for the interactions among grid averages in the grid-scale diffusion step. The change in grid average mixing ratios was applied to individual packets, which subsequently underwent subgrid diffusion, representing interaction between individual packets and the grid average mixing ratio.

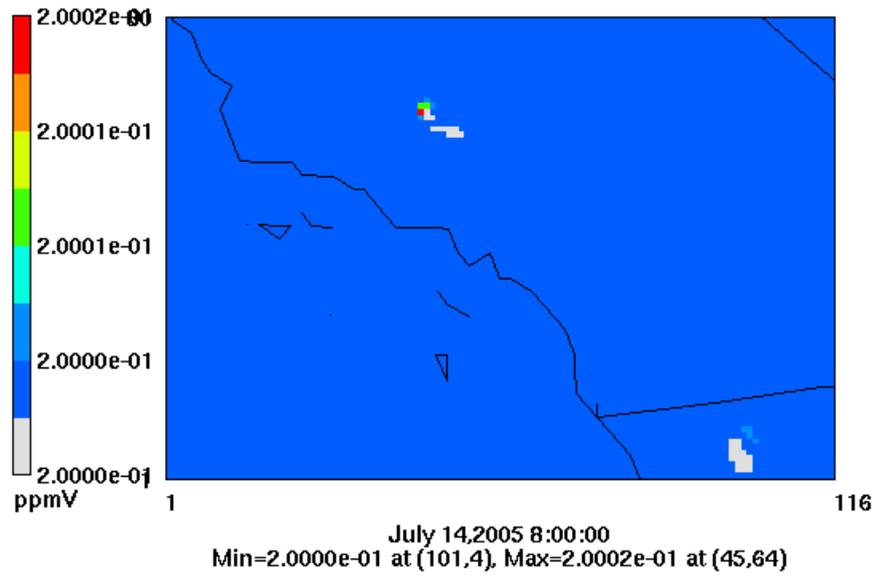
3.2 Behavior of CMAQ and CMAQ-TG-UH in a Simple Test Case

A simple test is devised to establish how well CMAQ and CMAQ-TG-UH conserves mixing ratio. Consider a tracer species that is not emitted, not deposited, and does not participate in chemistry. If the initial and boundary conditions are a constant mixing ratio everywhere in the domain, then that constant mixing ratio is expected to be maintained (Hu et al., 2006). In practice, however, inconsistencies between the meteorological model and the air quality model, e.g., different advection algorithms, time resolutions (MM5 output are provided in hourly intervals to CMAQ, which interpolates for intermediate time steps), may cause deviations from the constant mixing ratio for the tracer species, necessitating an adjustment step in the grid model after the advection calculation. CMAQ accounts for this inconsistency by advecting air density alongside gas species and using the ratio of the advected density and input density to correct the concentrations of gaseous species. Hu et al. (2006) noted that the adjustment step in CMAQ version 4.4 does not completely eliminate the mass inconsistency errors.

The transport-only test case was implemented by turning off dry deposition and emission in CMAQ in the corresponding extension files (GC_EMIS.EXT and GC_DEPV.EXT) and commenting out the chemistry routine in the source code (sciproc.F). CO was used as the tracer, with initial and boundary mixing ratios of 0.2 ppm throughout the domain. Results of the CMAQ simulation are shown in Figure 3-2. In this test case, CMAQ simulated a constant mixing ratio of 0.2 ppm to within 0.01%. This deviation from the expected constant mixing ratio was due to numerical errors introduced during the coupling, uncoupling, and mass adjustment steps.

A similar test was performed for CMAQ-TG-UH with the tracer CO (no chemistry, no deposition, no emissions). The CMAQ-TG-UH results are shown on the left side of Figure 3-3. CMAQ-TG-UH maintained the constant mixing ratio to within 1% during 16 simulation hours (hourly mixing ratios deviated from 0.2 ppm by as much as 3%). The deviations from the expected constant mixing ratio were also quite widespread.

Level 1



Level 10

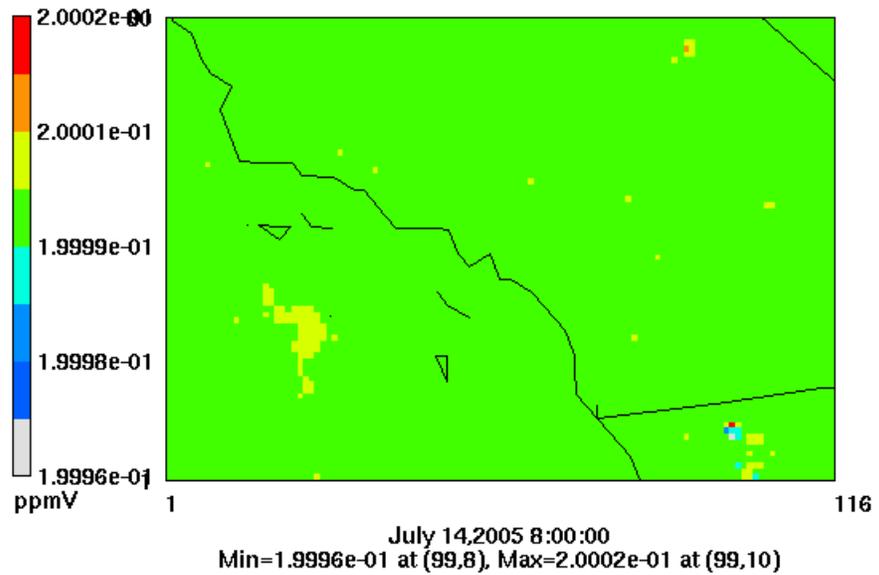


Figure 3-2. CO mixing ratio (16-hour average) for CMAQ with transport only (i.e., no emissions, no dry deposition, and no chemistry).

Mixing ratios of packets within a specific grid cell were tracked in a TG simulation to note the effects of transport processes in CMAQ-TG-UH:

- VDIFF: no change in number of packets, changes in mixing ratios
- ADVEC: possible change in number of packets, no change in mixing ratios for existing packets (new packets with different concentrations can be introduced into grid cell by advection)
- HDIFF: no change in number of packets, changes in mixing ratios.

In theory, the advection and diffusion of constant mixing ratio packets should always maintain that constant mixing ratio. The first deviation from the expected constant mixing ratios occurred in the horizontal diffusion step. In the UH implementation, the horizontal diffusion step was subdivided into grid-scale diffusion, subgrid diffusion, and a mass adjustment step. In this test case, changes due to mass adjustments were frequently larger than changes due to grid and subgrid diffusion. Based on comments within the source code file `adjmass.F`, this routine “adjust[s] packet mixing ratios to account for changes in air density over a synchronization time step. This is done to improve conservation of mass in the simulation of diffusion. It corresponds to the COUPLE-DECUPLE calls in the Eulerian version of CMAQ (not to ADJADV, which is unnecessary for TG)”. A ratio of the densities at the beginning and end of the time step was used to correct the mixing ratios of individual packets.

As discussed previously, the COUPLE-DECUPLE routines in CMAQ were essentially a pair of unit conversion steps from mixing ratio to a density (amount per volume) unit and back. With the ADJADV correction, CMAQ conserved both mixing ratio and species density (coupled units) during advection. By design, CMAQ-TG-UH also conserved mixing ratio in the advection step. CMAQ treated vertical diffusion in mixing ratio units but horizontal diffusion in the coupled units; while CMAQ-TG-UH treated diffusion in mixing ratios. No adjustment step was applied in CMAQ after horizontal diffusion. The forms of the horizontal diffusion equation were the same for both mixing ratio and coupled units. The coupled form can be written with spatial gradients of mixing ratios and a coupled eddy diffusivity (Byun and Schere, 2006). Therefore, the gradients in mixing ratios drive diffusion in both formulations using mixing ratios and using coupled units. By this analogy, the mixing ratio conservation

characteristics in the diffusion scheme in CMAQ-TG-UH should be as good as that in CMAQ. Therefore, the mass adjustment step after diffusion in the prototype CMAQ-TG-UH is unnecessary.

It should be noted that a scaling step was applied after TG advection in the original PMCAMx implementation (`advect_3d_rho.f`), where the concentration associated with a packet was scaled to reflect the change in density from the beginning time and location to the ending time and location along a trajectory. Chock et al. (2005) explained that this step assured that the species mixing ratios would not change as air parcels were transported. In CMAQ-TG, the mass correction was applied to the mixing ratios after the horizontal diffusion step while the advection step left the mixing ratio unchanged. The density correction involved only the density change in time at a particular location. The mass adjustment in CMAQ-TG-UH did not correspond to the density scaling in PMCAMx-TG not only because it changed the mixing ratios, but also because of the different densities used and its placement in the operator splitting sequence to correct the diffusion step.

Figure 3-3 shows the comparison of CMAQ-TG-UH with and without the mass adjustment step after diffusion. Without mass adjustment, CMAQ-TG-UH preserved mixing ratios several hundred times better. The mass adjustment step performed after diffusion may have created spurious diffusion in the UH implementation of CMAQ-TG-UH. The deactivation of the unnecessary mass adjustment step improved the mixing ratio conservation characteristics of CMAQ-TG-UH in a transport-only test case. The improved version without mass adjustment is hereafter referred to as CMAQ-TG.

3.3 Evaluation of Packet Management

Packet management is an important aspect of the TG approach. In theory, approximately one packet per grid cell should provide a resolution that is comparable to the grid-based approach. Multiple packets within a grid cell may offer additional resolution when the underlying terrain or flow pattern is complex. The default management scheme in the prototype CMAQ-TG is as follows:

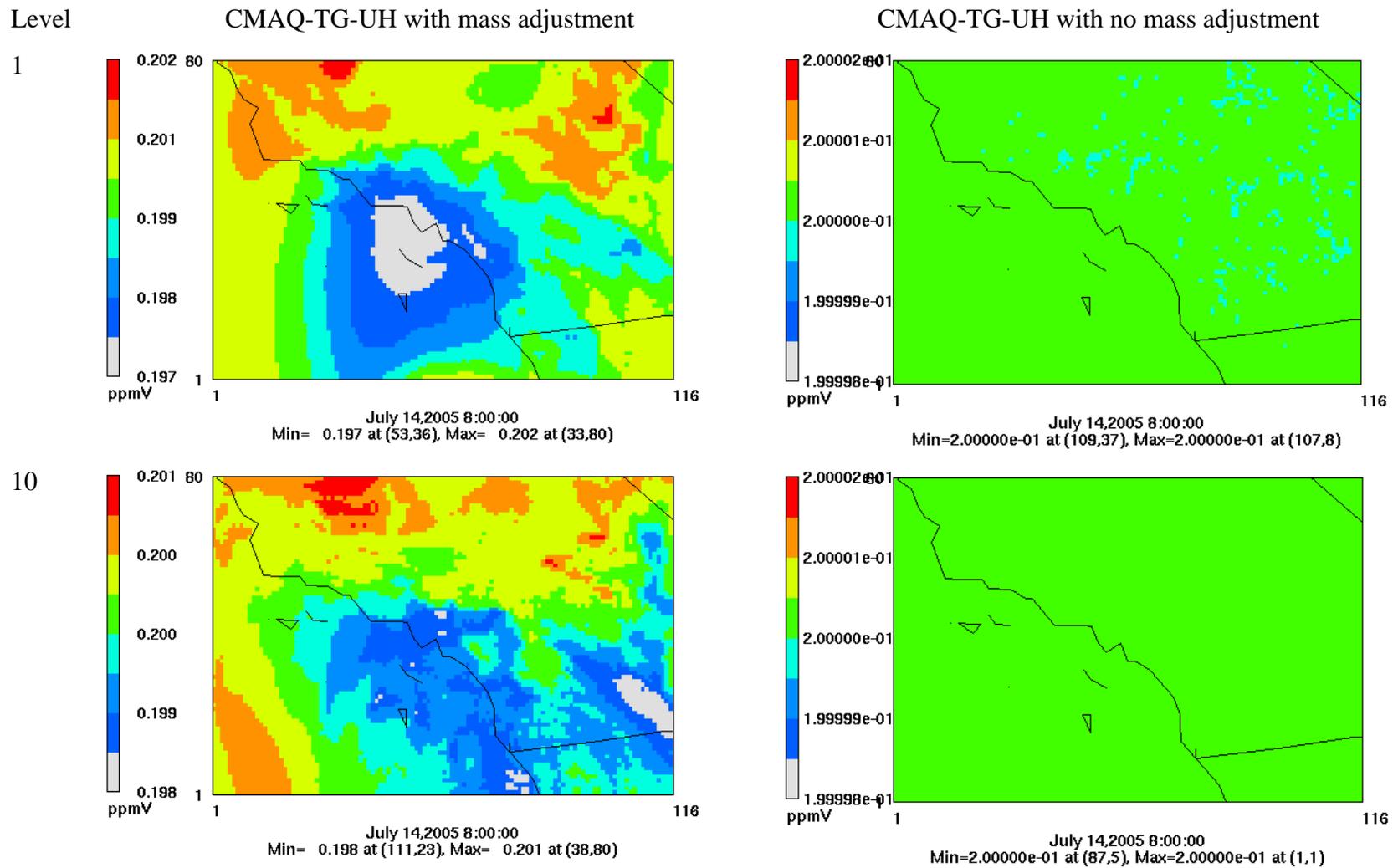


Figure 3-3. CO mixing ratio (16-hour average) for CMAQ-TG-UH simulations with transport only (i.e., no emissions, no dry deposition, and no chemistry) with and without mass adjustment.

- The 2 lowest layers are considered high resolution and are initialized with 4 packets in each cell
- Upper layers are initialized with only 1 packet in each cell
- Pruning, or the deletion of packets, takes place when the numbers of packets exceed 8 and 4, respectively, in high resolution and normal resolution cells
- After pruning is triggered, 4 and 2 packets, respectively, are kept in high and normal resolution cells
- Spawning, or the creation of new packets, takes place when no packet is left in a cell at any time step

For the test case domain, which contained 116 x 80 grid cells in the horizontal directions, the default scheme initialized the simulation with 37,120 packets in each of the 2 lowest layers and 9,280 packets in each of the upper layers. At the end of 16 hours of simulation, the high resolution layers lost packets (30,377 packets in layer 1 and 22,956 packets in layer 2), while the upper layers gained packets (approximately 20,000 packets). Many packets were spawned in 16 hours. For the lowest 4 layers, 25,829, 79,860, 97,095, and 65,203 new packets were generated, respectively. The 97,095 new packets spawned in layer 3 corresponded to one packet per grid cell every 1.5 hours.

Considering the entire domain, the total count of packets at the beginning of the simulation was 213,440. The total count of packets at the end of 16 hours was 360,587. However, the number of packets that were spawned over the period was 1,361,420, which implied that a large number of packets (1,214,273) were either pruned or advected out of the domain (Table 3-1). To evaluate the number of packets that were advected out of the domain, a simulation was conducted where pruning was turned off. The simulation without pruning suggested that 380,075 packets were advected out of the domain. Since the simulation was initialized with 213,440 packets, some level of spawning was absolutely necessary in this simulation. In the default case, an extra 587,804 packets were spawned because of pruning. Since information is lost when a packet is pruned, and this information cannot be regained when a new packet is spawned, a packet management strategy that minimizes pruning and subsequent spawning can potentially improve the accuracy of CMAQ-TG.

Table 3-1. Packet management in South Coast Air Basin test case

Total number of packets at all levels	Default	No Pruning Case
At the beginning of simulation	213,440	213,440
At the end of simulation	360,587	606,981
Spawned	1,361,420	773,616
Advected out of the domain or pruned ⁽¹⁾	1,214,273	--
Advected out of domain ⁽¹⁾	--	380,075

(1) total number of packets at hour 0 + total new packets – total number of packets at hour 16

4. EVALUATION OF TRANSPORT WITHIN CMAQ-TG

To study the transport characteristics of CMAQ-TG, simulations were performed with emissions (surface only) but without chemistry and deposition. The behaviors of the advection scheme and the diffusion scheme, as implemented by UH, were alternatively studied by turning off the other process. (Post diffusion mass adjustment was not used for these CMAQ-TG simulations.)

Figure 4-1 shows the results of a CMAQ simulation and a CMAQ-TG simulation without vertical and horizontal diffusion. With only advection and emission, mixing ratios of the inert CO species at the surface were much greater in the CMAQ-TG case than in CMAQ. Moreover, the smooth spatial distribution predicted by the CMAQ advection-only simulation was a result of artificial diffusion due to artificial dilution in the volume of the grid cell and numerical diffusion associated with the PPM advection scheme (Pun et al., 2006); both types of artifacts were avoided in the Lagrangian TG advection scheme. The grainy appearance of the CMAQ-TG spatial distribution reflected the relative lack of numerical diffusion. The TG advection scheme also predicted significantly higher domain maximum mixing ratios of CO at the surface compared to the PPM scheme.

Advective transport during the first 8 hours of simulation contributed to mixing ratios of CO above background in upper levels. Figure 4-1 shows that in the absence of physical diffusion, CMAQ-TG predicted higher mixing ratios reaching layer 5 than CMAQ (Figure 4-2). Areas showing above-background mixing ratios were also much more limited in spatial extent in the CMAQ-TG simulation. Therefore, numerical diffusion in CMAQ-TG is also noticeably less than in CMAQ in the vertical direction. These results confirm that the TG approach is inherently less diffusive than the PPM scheme in the stock CMAQ version.

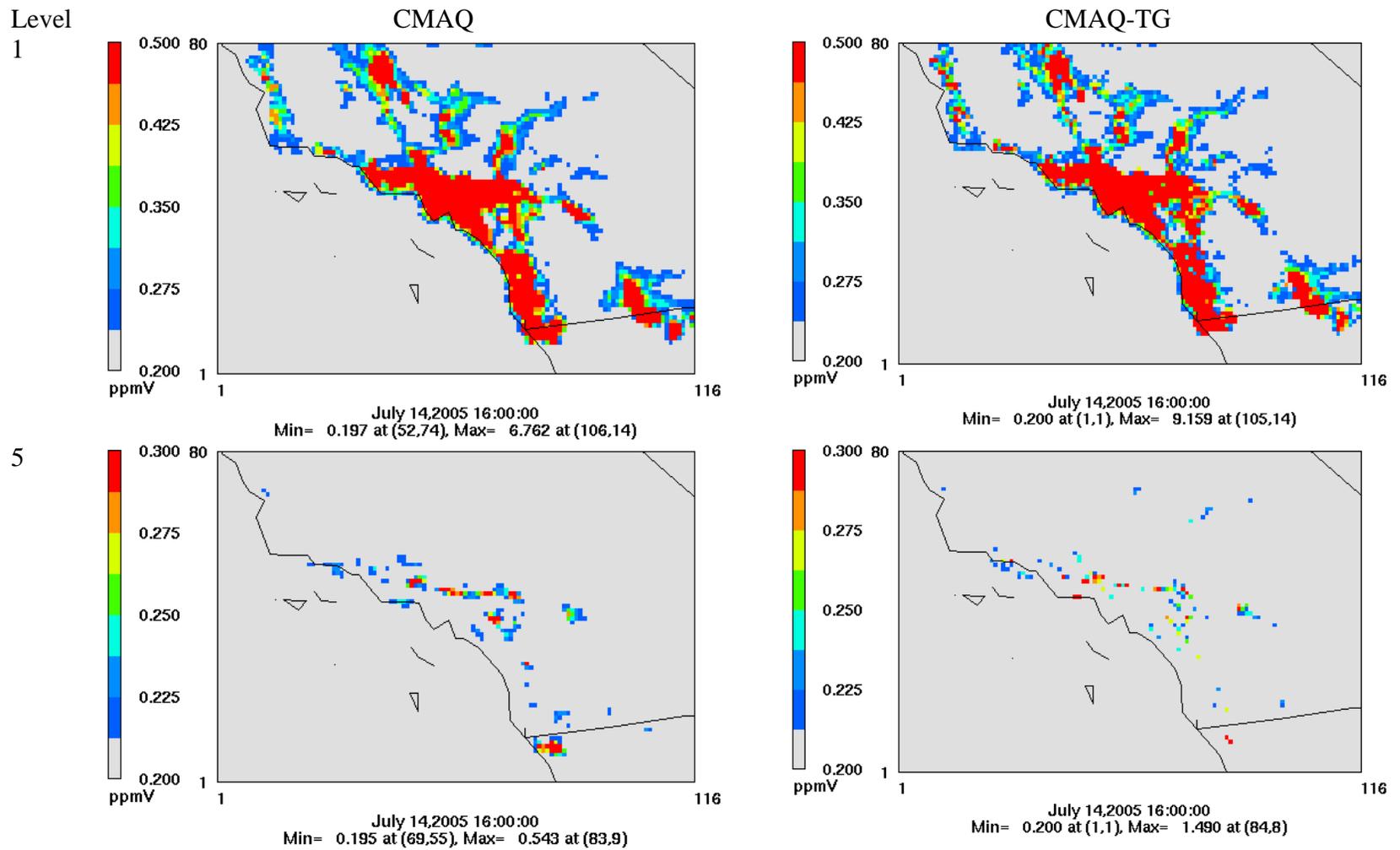


Figure 4-1. CO mixing ratio at hour 8 (16 GMT) for CMAQ and CMAQ-TG simulations with advection and emission only (i.e., no diffusion, no dry deposition, and no chemistry). Note different scales for level 1 and level 5.

To test the importance of diffusion in distributing pollutants in the test case, simulations were carried out with emissions and diffusion only, but no advection. Chemistry and dry deposition continued to be deactivated. When the horizontal and vertical diffusion processes interacted with emission only, both CMAQ and CMAQ-TG produced very similar results, as shown in Figure 4-2. At the surface, CMAQ tended to simulate slightly higher mixing ratios than CMAQ-TG near the sources of the CO plumes. The domain maximum surface mixing ratios in Figure 4-2 provide some quantification of the difference (<1%). The difference appears to be due in part to the different time steps used in these two models. At higher altitudes, the CO distributions in CMAQ and CMAQ-TG due to diffusion of surface emissions appeared quite similar, and much more widespread than in the advection-only case (Figure 4-1). The similarity of the diffusion predictions is to be expected, because CMAQ-TG uses the same algorithm as CMAQ to calculate the diffusion coefficient among different grids. The UH diffusion scheme applies the diffusion calculation to individual packets within the grid to represent their interaction with neighboring grid average mixing ratios. When advection is switched off, the packets remain at the same locations throughout the simulation, and none of the other processes caused any subgrid scale variability among packets. Therefore, subgrid scale diffusion has no effect on a diffusion-only simulation (no mixing ratio gradient within a given grid cell) and the UH diffusion treatment defaulted to the CMAQ treatment except diffusion is applied to packets rather than grid mixing ratios. Therefore, physical diffusion was an important process for moving surface pollutants to upper levels in this test case.

The TG advection module within CMAQ is subject to less artificial diffusion than traditional grid-based advection module. As a numerical scheme, TG is not subject to numerical diffusion like traditional advection solvers. In addition, the transport of pollutants takes place within the confines of single packets along a trajectory, rather than the volume of the grid cell, minimizing the artificial dilution due to the lack of spatial resolution. However, an advection scheme that is numerically less diffusive does not necessarily translate into less diffusive spatial distributions for inert species in an air

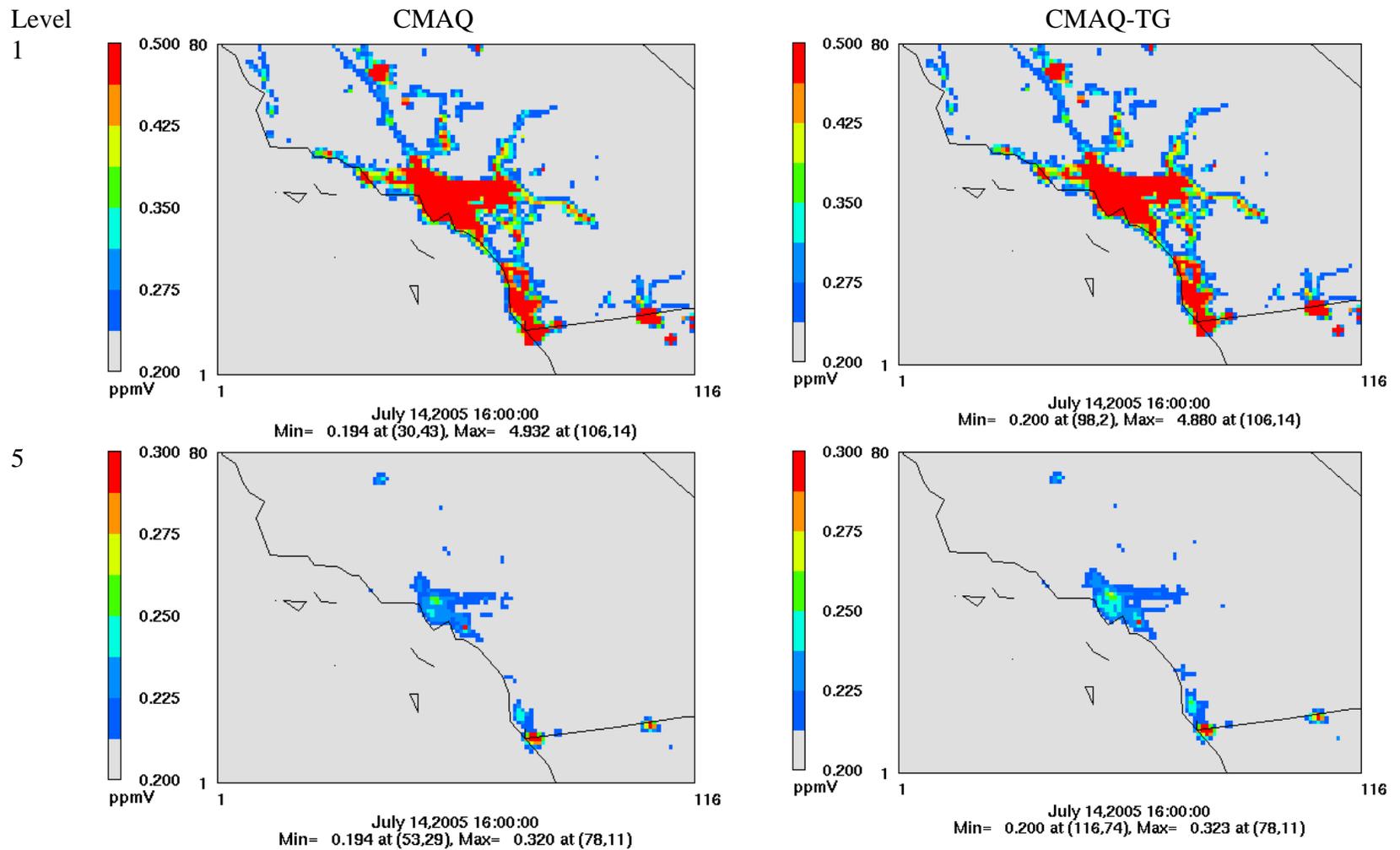


Figure 4-2. CO mixing ratio at hour 8 (16 GMT) for CMAQ and CMAQ-TG simulations with diffusion and emission only (i.e., no advection, no dry deposition, and no chemistry). Note different scales for level 1 and level 5.

quality simulation. The physical diffusion module, which is formulated based on gradients of concentrations, may well play a significant role in dispersing concentrations. The previous test case showed that when advection was turned off, the UH grid diffusion routine implemented within CMAQ-TG showed similarities when compared to the CMAQ routine. In the next section, aspects of the diffusion scheme within CMAQ-TG are investigated further when interaction with the Lagrangian advection process are allowed.

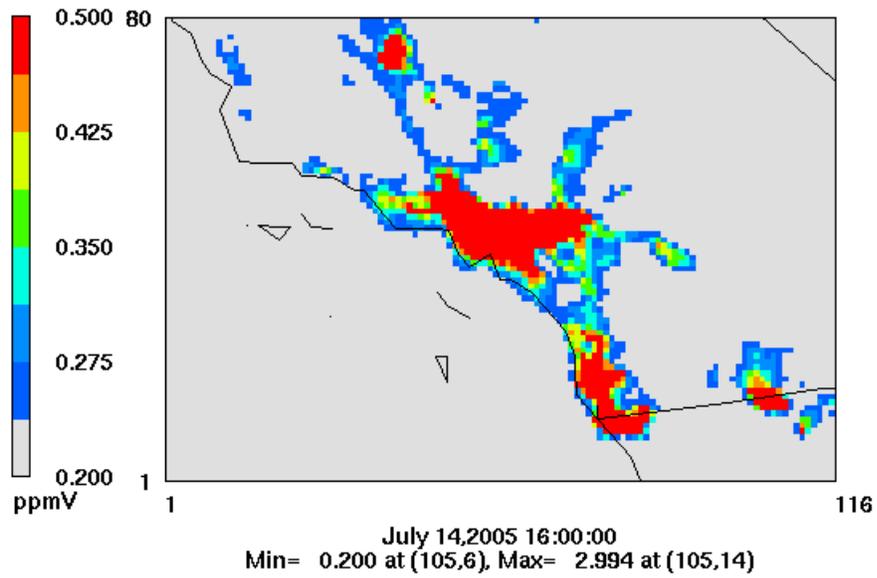
It should be noted that how best to represent turbulent diffusion in an Eulerian model that takes advantage of the Lagrangian approach for advection is an open science question. The impacts of different formulations of diffusion on simulated mixing ratios are illustrated using 3 different simulations with emissions, advection and diffusion (no chemistry, no dry deposition). The results of the original UH diffusion implementation are provided as a reference in Figure 4-3.

As discussed previously, the treatment of diffusion associated with the Lagrangian advection module involved a grid and a subgrid component, In the original diffusion module described in Chock et al. (2005) for PMCAMx, for a packet i ,

$$C_i^{new} = C_i^{old} + \Delta C_D + \Delta C_{SD,i} \quad (2)$$

the grid diffusion (ΔC_D) step handled interactions between grid-average mixing ratios (same of all packets i within the grid cell), while the subgrid diffusion step represented the interactions between packets within a given cell and altered the range of packet mixing ratios within that grid cell. The UH implementation of diffusion was different. Grid diffusion was represented by the interaction of individual packets within a cell and average grid mixing ratios in nearby cells. This grid diffusion formulation calculated $\Delta C_{D,i}$ for each packet (instead of one ΔC_D for all packets within a grid cell) and can reduce the range of mixing ratios within a grid cell. Subgrid diffusion was modeled based on the subsequent gradient of mixing ratios between an individual packet and the cell-average mixing ratio, and was quite similar to the PMCAMx step. Because the grid diffusion step altered individual packet mixing ratios based on separate calculations, the subgrid diffusion may be somewhat redundant in the UH diffusion scheme. The first test

Level 1



Level 5

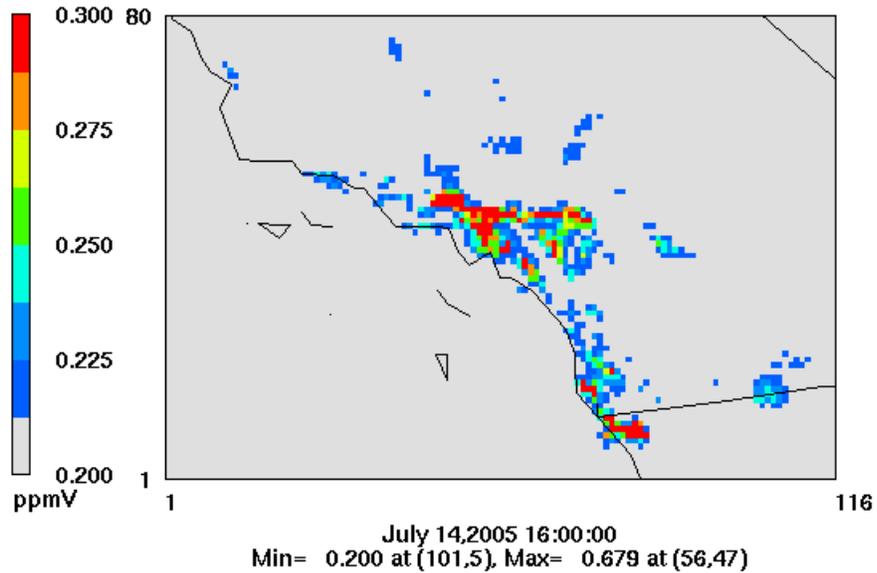


Figure 4-3. CO mixing ratio at hour 8 (16 GMT) for a CMAQ-TG simulation with transport and emission only (i.e., no dry deposition, and no chemistry), using the implementation of horizontal and vertical diffusion by UH. Note different scales for level 1 and level 5.

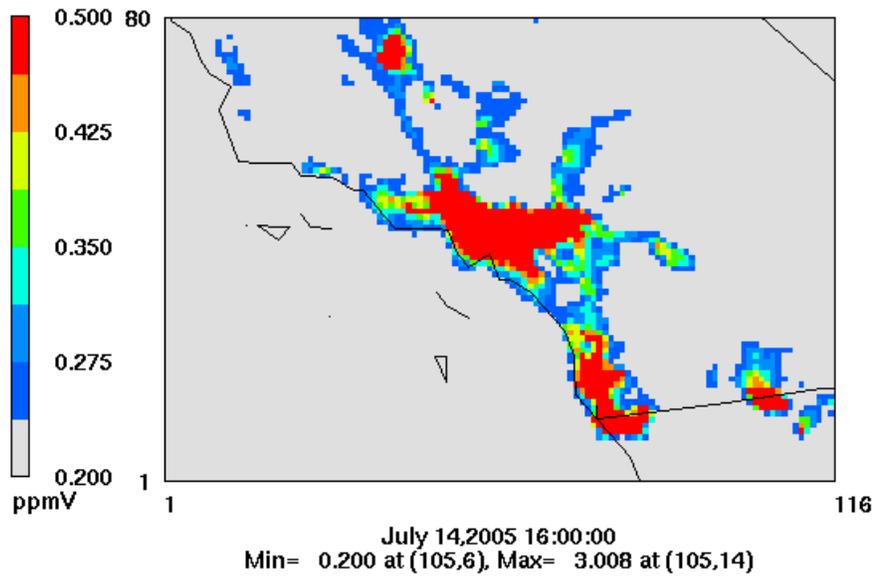
was to evaluate the effect of the extra subgrid diffusion in the UH scheme by turning off the subgrid diffusion process. Figure 4-4 shows the results of this simulation. The extra subgrid diffusion seemed to cause only a small change in the simulated mixing ratios.

The sensitivity of simulated mixing ratios to the diffusion treatment was further illustrated by the implementation of a scheme similar to Chock et al. (2005) for the calculation of grid diffusion in the horizontal and vertical directions. In this scheme, the diffusion algorithm of CMAQ was used to calculate the change in the grid average mixing ratios. Mixing ratios of individual packets were adjusted according to the required mixing ratio change. The results shown in Figure 4-5 show a fairly significant difference (20%) of the peak mixing ratio at the surface level compared to the UH diffusion scheme (Figure 4-3), although differences in upper levels tended to be smaller.

The above examples show a range of behavior associated with various treatments of diffusion in conjunction with a Lagrangian advection scheme such as TG. In addition, there are uncertainties in the parameterization of diffusion coefficients even in a traditional Eulerian approach. As an example, Figure 4-6 shows the results of a CMAQ-TG simulation where the modeled diffusivities in the UH diffusion scheme were reduced by a factor of 10. Compared to Figure 4-3, reducing the diffusivities had the obvious effect of lowering dispersion, resulting in higher domain maximum concentrations in surface and aloft layers. The maximum mixing ratios in layer 1 and layer 5 were closer to the advection-only simulation (Figure 4-1) in the reduced diffusivity case.

The Lagrangian TG advection scheme allows the investigation of the diffusion algorithms free from the confounding effects of numerical diffusion and grid cell dilution.

level 1



level 5

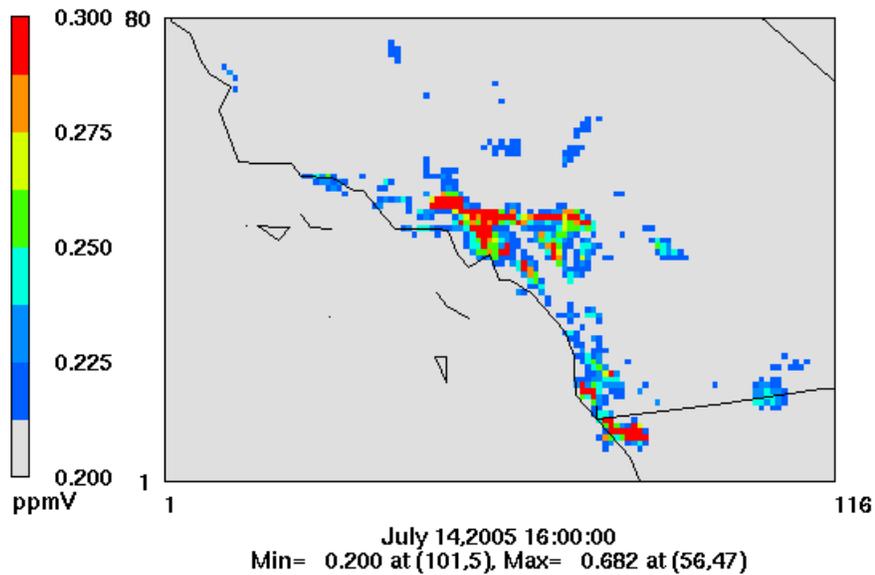
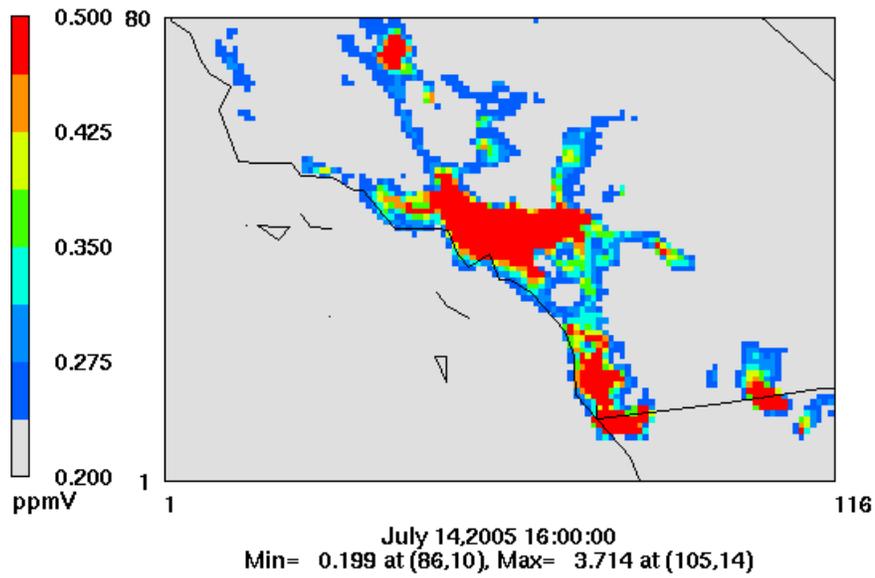


Figure 4-4. CO mixing ratio at hour 8 (16 GMT) for a CMAQ-TG simulation with transport and emission only (i.e., no dry deposition, and no chemistry), using the implementation of diffusion by UH for grid diffusion only (subgrid diffusion deactivated). Note different scales for level 1 and level 5.

level 1



level 5

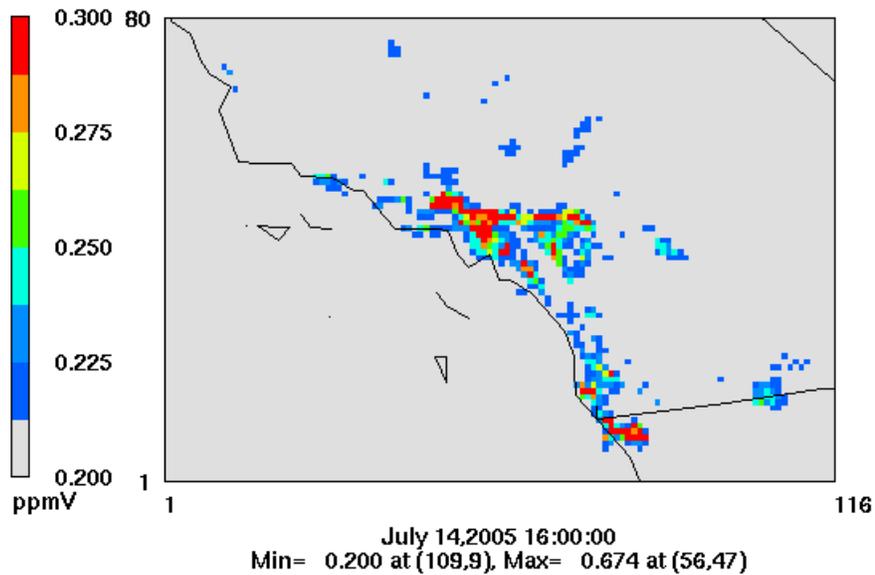
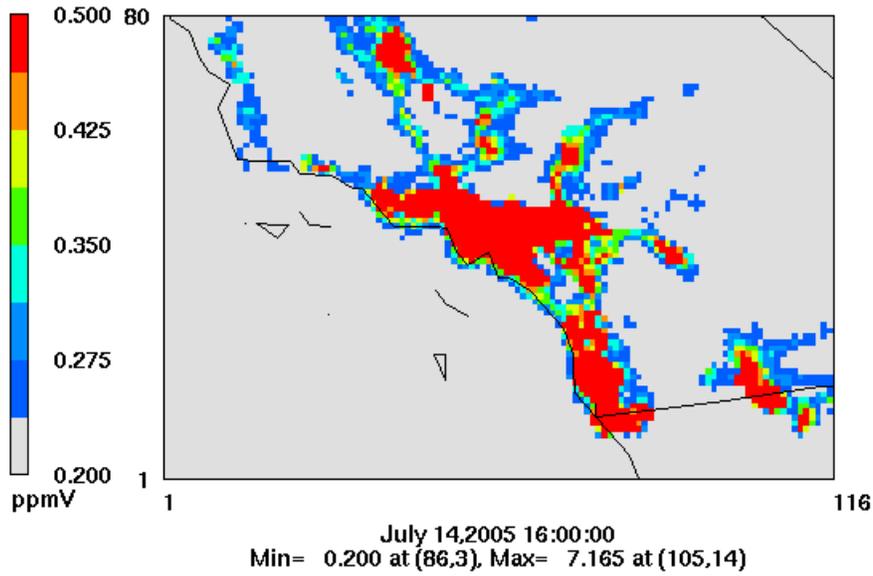


Figure 4-5. CO mixing ratio at hour 8 (16 GMT) for a CMAQ-TG simulation with transport and emission only (i.e., no dry deposition, and no chemistry), using the implementation of a diffusion scheme similar to Chock et al. (2005) for grid and subgrid diffusion. Note different scales for level 1 and level 5.

Level 1



Level 5

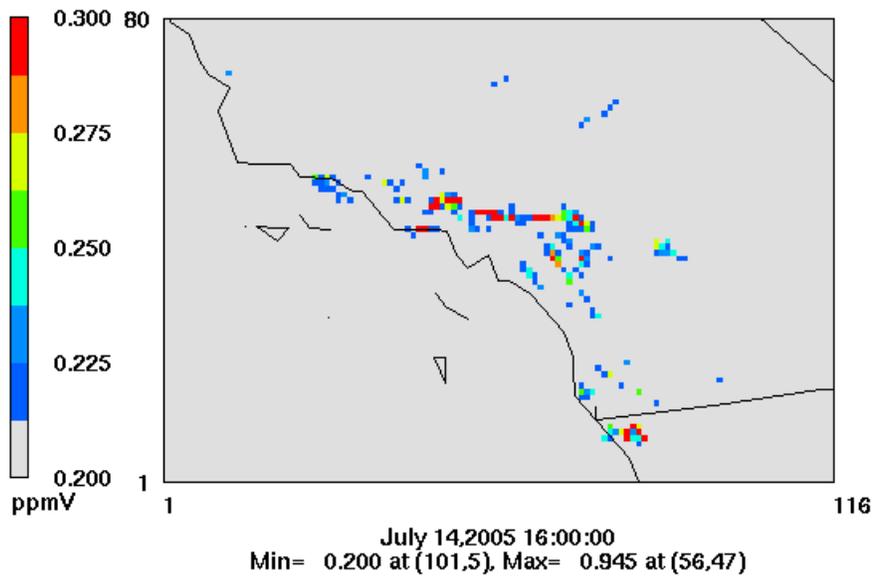
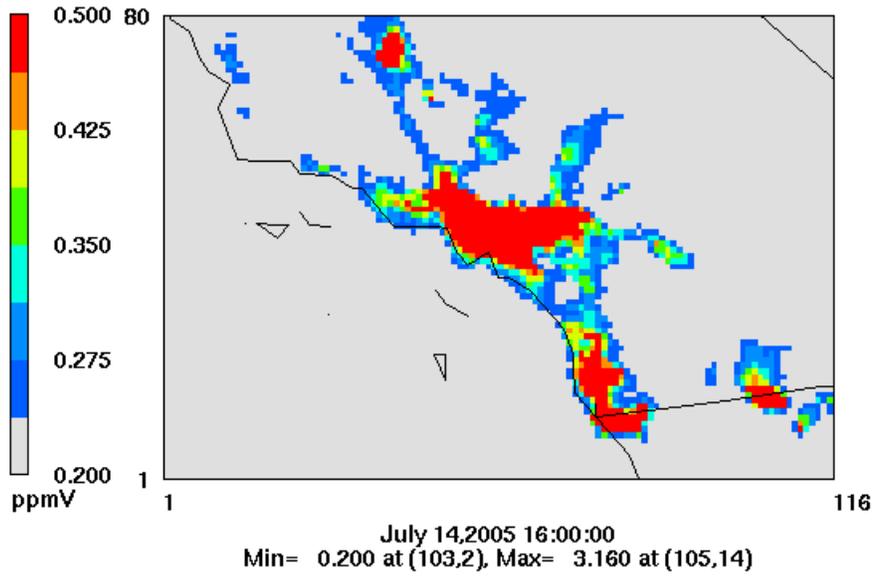


Figure 4-6. CO mixing ratio at hour 8 (16 GMT) for a CMAQ-TG simulation with transport and emission only (i.e., no dry deposition, and no chemistry), using an alternative diffusion treatment based on the UH implementation with lower horizontal and vertical diffusivity. Note different scales for level 1 and level 5.

5. ALTERNATIVE PACKET MANAGEMENT

As noted in Section 3.3, a packet management scheme that minimizes pruning and the subsequent spawning of packets may improve the accuracy of CMAQ-TG. A TG simulation with no pruning of packets was run to evaluate the effects on the predicted mixing ratio and spatial distribution of an inert tracer (no chemistry, no deposition). Results of this simulation are shown in Figure 5-1. Except for the packet management scheme, the advection and diffusion treatments were identical to the base case shown in Figure 4-3. At hour 8 of the simulation, the case without pruning simulated a higher domain maximum CO mixing ratio in layer 1 than the default management strategy. The largest difference (up to 0.6 ppm) between the default and no-prune cases occurred near the point with the highest mixing ratios. The overall spatial distribution of CO in layer 1 appeared quite similar and did not show appreciable differences in the dispersion characteristics. Upper level mixing ratios were driven primarily by transport from the surface in this test case. Because upper level mixing ratios are represented by fewer packets per grid cell on average, they are expected to be more sensitive to packet management strategies than surface mixing ratios. For level 5 predicted mixing ratios could also differ by as much as 0.6 ppm at a given time and location, which was a larger fractional difference due to lower mixing ratios in upper levels. The difference varied with time and did not seem to represent a systematic effect. Therefore, the prediction of vertical transport may be sensitive to the management of packets in a CMAQ-TG simulation.

Level 1



Level 5

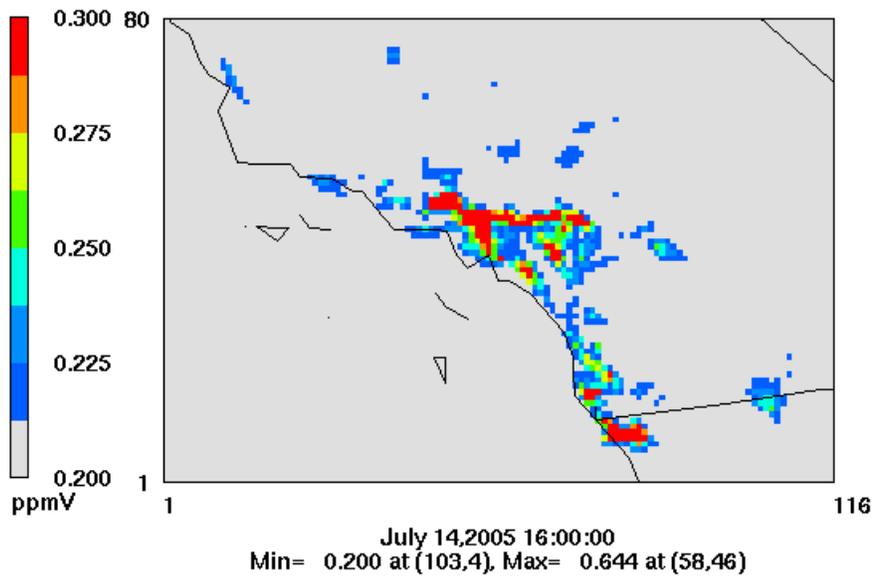


Figure 5-1. CO mixing ratio at hour 10 (18 GMT) for a CMAQ-TG simulation with transport and emission only (i.e., no dry deposition, and no chemistry), using an alternative packet management strategy without pruning. Note different scales for level 1 and level 5.

6. CONCLUSIONS

The TG advection scheme implemented in CMAQ version 4.4 is considerably less diffusive than traditional grid-based advection solvers, such as the PPM scheme.

Deactivating a mass adjustment step performed after horizontal diffusion allowed CMAQ-TG to conserve mixing ratios in a simulation with constant initial and boundary conditions. CMAQ-TG results were somewhat sensitive to the strategy used for packet management, especially for upper level mixing ratios that were represented by relatively few packets within each grid cell. The overall spatial patterns of an inert pollutant did not indicate a systematic change in dispersion characteristics due to packet management strategies. When both advection and diffusion processes affect mixing ratios of an inert species, the simulation of physical diffusion may compensate for the lack of artificial diffusion in the TG advection scheme and lead to a dispersive mixing ratio field in a simulation of an inert tracer. In the South Coast test case, physical diffusion played a significant role determining the distribution of pollutants in a CMAQ-TG simulation. Several implementations of diffusion schemes showed a range of results, indicating the sensitivity of CMAQ-TG predictions to the representation of physical diffusion. Treatment of diffusion is considered an open science question. Because of the confounding effects among physical diffusion, artificial diffusion and grid cell dilution in a traditional Eulerian air quality model, the diffusion module has seldom undergone rigorous evaluation. In addition to parameterizations of the type used in CMAQ, Lagrangian particle dispersion models have also been proposed. The TG advection scheme that is relatively free of numerical artifacts provides an opportunity for future investigations into the behavior of the diffusion schemes.

7. ACKNOWLEDGMENTS

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