Effects of Sub-Grid Scale Terrain upon CAMx Air Quality Simulation.

Carlie J. Coats, Jr.*^{1,} M. Talat Odman² and Saswatti Datta¹

¹Baron Advanced Meteorological Systems, LLC., Raleigh NC, USA ²Department of Environmental Engineering, Georgia Institute of Technology, Georgia, USA

Statement of the Problem

Meteorology models typically "smooth" the underlying terrain for spatial scales of at least 3 dx, in order to avoid the formation of spurious waves due to 2 dx features interacting with advection schemes. For MM5, the minimum terrain smoothing permitted is 3 dx averaging, so that a nominal 4 KM grid spacing actually corresponds to the use of 12 KM averaged terrain height. This smoothing causes errors at the grid scale, particularly for such meteorology fields as surface temperature. Moreover, conventional meteorology models assume a laminar atmosphere that does not simulate sub-grid scale effects caused by terrain variability. In this case study, we examine some of the sub-grid scale effects upon air quality processes, particularly emissions and dry deposition. We do not study the effects of grid scale terrain height error, nor the effects of sub-grid scale terrain variability upon wet deposition. It is also beyond the scope of this study to modify meteorological model dynamics (where meteorology model drag should be enhanced to account for orographic drag, etc., as is done in ECMWF).

In this study, we implemented a sub-grid scale parameterization within the CAMx air quality model; the effects for a 4 KM California domain upon CAMx simulations are the subject of an accompanying paper with lead author Saswati Datta. We begin with a terrain preprocessor **PENFRAC** that evaluates both the grid scale error (due to smoothing in MM5's **TERRAIN** program) and the sub-grid scale terrain variability in terrain heigh. Within CAMx, we implement parameterizations for sub-grid scale terrain effects upon surface emissions, point source emissions, and dry deposition, it being outside the scope and the data-availability of the project to be able to re-run meteorologically dependent (biogenic and mobile source) emissions with corrections for the surface temperature errors due to MM5 terrain smoothing. Other studies have shown that the grid scale errors in MM5 terrain can lead to significant errors in biogenic emissions. Failure to model the sub-grid scale effects we study in "vanilla" CAMx (and other air quality models) leads to vertical mis-allocation of emissions and dry deposition. It should be noted that there are further effects due to the interaction of this mis-allocation with transport and diffusion.

Model Implementation:

Sub-Grid Terrain Analysis Pre-Processor

Terrain analysis is performed by pre-processor program **PENFRAC** that reads in 30-arc-second (approximately 0.7 KM) digital elevation model (DEM) terrain data in Models-3 I/O API format, derived from the same USGS generated DEM data used to drive *Mode 6* of program **TERRAIN**. This program creates two files:

HT_2D with these terrain related 2-D variables:

HTMIN, minimum of DEM terrain heights in grid cell (M) *HTBAR,* mean of DEM terrain heights in grid cell (M) *HTMAX,* maximum of DEM terrain heights in grid cell (M) *HTSIG,* standard deviation of DEM terrain heights in grid cell (M) HT_3D with 3-D variable:

TFRAC, the fraction of each horizontal grid cell in contact with each 3-D model layer.

Note that *HTBAR* can be used to evaluate grid scale errors in meteorology model terrain, and that *HTMAX-HTMIN* and *HTSIG* are two different measures of the terrain variability within each grid cell. In this study, we used the "simple-Z" version of **PENFRAC** which uses MM5 layer thicknesses and a base elevation *HTBAR-HTSIG* to construct a 3-D layer system. Terrain penetration fraction *TFRAC* is constructed by counting how DEM elevation-points in each met-grid cell are related to this 3-D layer system, subject to the constraint that DEM-values below model-bottom are counted as being in Layer 1.

Sub-Grid Scale Terrain Effects in CAMx

We have implemented three classes of sub-grid scale terrain effects as modifications to CAMx Version 4.31:

- Dry-deposition effects
- Surface-emissions effects
- Point-source emissions effects

For the first two of these, the implementation uses TFRAC from **PENFRAC's** HT_3D to deal with vertical re-allocation effects; the latter uses high resolution DEM CRO 2D data to construct stack-height corrections (subject to the constraint that stack-top may not be below bottom-of-model). The implementation adds a new Fortran module **LPEN MOD** that encapsulates reading and processing these files, particularly the nest management, the re-aggregation of TFRAC from the native MM5 lavers to the variable LFRAC on the collapsed CAMx layers. and the adjustment of stack height for high resolution DEM terrain. These terrain parameterization effects may be turned off by means of environment variables at program-launch, following the conventions of Models-3.

Routine **DIFFUS** was modified so that it calls **LPEN_NEST** to activate **LPEN_MOD** for the current grid. Then within its internal time step loop it alternates between calling diffusion-kernel **VDIFFIMP** and computing 3-D mass exchanges from the concentration field to the deposition field, using LFRAC as the weights for accumulating mass from the model layers. The effect is that for significantly variable terrain, dry deposition fractionally removes mass from several layers of the atmosphere. In the day-time mixed regime, the differences are insignificant; however, during stable periods (as at night), the scheme partially scavenges multiple layers rather than completely scavenging Layer 1 only, generating greater dry deposition totals and more realistic end-of-night concentration profiles.

As we implemented this dry deposition parameterization, we discovered that the original CAMx scheme had a mass inconsistency, where first dry-deposition was treated as a bottom boundary condition sink in **VDIFFIMP** and then separately computed for output from post-**VDIFFIMP** Layer 1 concentrations. The effect of this mass inconsistency was to introduce a mild low bias into the dry deposition field relative to the modeled concentrations.

Routine EMISS was modified to call LPEN_NEST, then to allocate each grid cell's emissions in the vertical using *LFRAC* as weights. Routine PLUMERIS uses terrain adjusted stack heights as the basis of its plume rise computation. Again, effects are most marked in the stable nocturnal boundary layer, where vertical allocation may have substantial effects upon nocturnal precursor transport; unstable-regime effects are much smaller.

In the process, the CAMx code was extensively re-parallelized, raising the parallel efficiency on 8 SGI Origin processors from about 35% to better than 95%. The build-system was modified to support PathScale, Intel, and Sun compilers for Linux. Also, a number of additional optimizations relating to superfluous arraycopy operations in VDIFFIMP were performed, increasing the single-processor performance of the code noticeably. However, there are still many opportunities for further code speedup. These code modifications were supplied back to the California Air Resources Board.

Terrain Analysis for the CCOS Domain

Plots for a terrain analysis based on the *MM5* **MMOUT** file for this case are given by the figures in the *Appendix* at the end of this paper. Figure 1 shows the extent of the domain, while plotting the "true mean" terrain height computed directly on this 4-KM grid from USGS 30-second digital elevation model (DEM) data. Figure 2 shows the MM5 error in terrain elevation due to smoothing in the TERRAIN program. Figure 3 shows the range of terrain elevation (from max to min of the DEM within each grid cell), on a "raw" PAVE scale. Figure 4 shows the maximum layer of terrain penetration, which ranges up to Layer 22 at one point (representing an elevation difference of about 1000 meters). Figures 5-8 show the fraction of each cell that Simple-Z regards as being in contact with Layers 1, 2. 5. and 10 of the atmospheric model. respectively. To get the fraction of the cell that interacts with a given layer L > 1 for purposes of emissions or dry depositions, one computes the difference

LFRAC(L) - LFRAC(L+1)

Note that terrain penetration is significant through layer 10 or so, and is quite small (particularly as regards emissions and pollutant distributions) for layers 15 or higher. Note also that the effects are insignificant in the central San Joaquin Valley, but are substantial in the foothills and the mountains that surround it-in particular, for transport between it and the San Francisco Bay area.

Acknowledgements

This work was funded under the Central California Ozone Study's request for proposals, "Improve Conservation of Mass Module in Air Quality Models".

The statements and conclusions of this report are those of tine Investigator, and not necessarily those of the California Air Resources Board, the San Joaquin Valleywide Air Pollution Study Agency, or its Policy Committee, their employees or their members. The mention of commercial products, their source, or their use in connection with material reported herein is not to be construed as actual or implied endorsement of such products.

References

Coats, C. J., A Conservative Framework for Sub-Grid Scale Terrain Effects in Air Quality Forecast Models. *7th Conference on Atmospheric Chemistry*, American Meteorology Society, San Diego CA Jan. 2005.

Coats, C. J., SMOKE R&D for Sub-Grid Scale Terrain Effects and Air Quality Forecast Modeling. Presentation for *US EPA ORD*, RTP, NC. Feb. 2005. Available at URL *http://www.baronams.com/staff/coats/EPA_feb2* 005.ppt

Coats, C. J., SMOKE-RT Development for WRF-Chem and Air Quality Forecasting. *4th Annual CMAS Models-3 Users' Conference* UNC-Chapel Hill, Chapel Hill, NC, September 26-28, 2005. Available at URL *http://www.baronams.com/staff/coats/CMAS_wrf _smoke_2005.pdf*

Appendix : Terran Analysis



Figure 1: Terrain height computed by directly averaging USGS 30-second Digital Elevation Model (DEM; approximately 0.7 KM) terrain heights over each 4KM grid cell



Figure 3: Range of terrain height: *HTMAX – HTMIN* for 30-second DEM elevations within each 4 KM grid cell. Note that max range is 2071 meters...

MM5 terrain height error HTERR = HTBAR - HT (meters) Computed using 30° USGS DEM averaged over each 4KM grid cell



Figure 2 : Error in *MM5* terrain height due to the smoothing in the *MM5 TERRAIN* preprocessor.



Maximum Terrain penetration layer MXPEN

Simple-Z sub-grid scale parame

Figure 4: Maximum terrain penetration layer for the 4 KM *MM5* grid, using the Simple-Z sub-grid scale terrain parameterization. The maximum of layer 22 corresponds to an elevation of approximately 1000 meters.



Figure 5: Fraction *TFRAC* of each 4 KM grid cell that should be regarded as being "within layer 1" as computed by the *Simple-Z* sub-grid scale terrain penetration parameterization



Figure 6: Layer 2 TFRAC



Figure 7: Layer 5 TFRAC

Layer 10 Terrain Penetration Fraction TFRAC Simple-Z sub-grid scale parameterization



Figure 8: Layer 10 TFRAC