Comparison of Subgrid Turbulence Closure Schemes in WRF/Chem

Evelyn D. Grell[1,2], Jian-Wen Bao[1], Sara A. Michelson[1,3], Georg A. Grell[1,3]
Stuart A. McKeen[1,3] and Bright Dornblaser[4]

[1]NOAA Earth Systems Research Laboratory, Boulder, CO
[2]Science and Technology Corporation, Hampton, VA
[3]CIRES, University of Colorado, Boulder, CO
[4]Texas Commission of Environmental Quality, Austin, TX

1. Introduction

Observations have shown that small variations in surface meteorological conditions can have a dramatic effect on the spatial and temporal characteristics of high surface ozone concentrations (MacDonald and Roberts 2002). These ozone maxima are extremely difficult to simulate, yet can play an important role in the air quality. Contributing to this difficulty is the uncertainty in simulating the turbulent mixing caused by large-sized eddies in the daytime atmospheric boundary layer.

In a typical WRF model run, sub-grid mixing is parameterized within the boundary layer physics. It is assumed that there is a clear scale separation between the horizontal and vertical mixing, and vertical mixing is dominant. This assumption may not be valid when horizontal grid spacing approaches 1 km or less, and a fully three-dimensional subgrid turbulence closure should perhaps replace the parameterized mixing (Wyngaard 2004).

We present results from a case study in which 200m grid spacing is used, and three different options for vertical mixing are tested. The explicit diffusion option is applied with eddy viscosities determined using two different closure schemes, and a more conventional model set-up in which the Mellor-Yamada-Janjic boundary-layer parameterization is also applied. The impact of these various closures on the transport and reaction of chemical constituents as well as on the meteorological fields is analyzed.

2. Methodology

The coupled WRF-chemistry model (Grell et al. 2005) is run on multiple meshes using one-way nests of resolution 36km, 12km, 4km, 1km, and 0.2km, centered over Houston, Texas. On the 0.2km grid, 241x201 grid points are used, with 51 vertical levels. The Noah land-surface model and the Monin-Obukhov surface layer schemes are utilized to provide surface forcing. Online chemistry is computed using the RADM2 mechanism.

A case study from the Texas Air Quality Study 2000 (TEXAQS 2000) is used to provide realistic initial and boundary conditions for a clear day case in which the strength of the urban heat island modifies the evolution of the sea breeze, and thus impacts the air quality in the Houston region. Simulations for the coarser grids (1km and greater) were 24 hours in length, beginning at 0000 UTC 25 August 2000. Because of the large amount of computing resources required by the 0.2 km simulations, these were initialized at 1200 UTC 25 August 2000 and run for only 10 hours. This time period (7 am to 5pm local time) covers the evolution of the daytime atmospheric boundary layer (ABL) from a shallow, stably stratified layer to a deep, well-mixed layer and includes the onset of the sea breeze in the late afternoon.

The chemistry is based on point source emissions only. The impact of clouds on the radiation and photolysis is removed in order to simplify the comparison of model results.

For vertical diffusion, 3 different options are tested:

1) the Smagorinsky closure (diff_opt=2, km_opt=3),

2) the prognostic turbulent kinetic energy (TKE) closure (diff_opt=2, km_opt=2), and

3) the Mellor-Yamada-Janjic (MYJ) boundary layer scheme (diff_opt=1, km_opt=4).

These schemes result in different determinations of the horizontal and vertical eddy viscosity coefficients (K_h, K_v).

Although the sub-grid scale (SGS) options (1) and (2) above exist in the standard release version of WRF, they were not coupled with the temporally and spatially varying surface heat and momentum fluxes computed by the land-surface model. Our first task was to include these fluxes in the lower boundary condition of the two SGS closures, as well as in the buoyancy and shear production terms of the TKE equation.

3. Results

Fig. 1 shows the domain used for the 0.2 km simulations, overlaid with the simulated winds at 2200 UTC. Also displayed are the concentrations of NO_x, the sum of NO and NO_2. Because NO_x is rapidly being converted to ozone at this time, the concentrations are relatively low, with higher amounts found only near the emission sources.

Galveston Bay and the Gulf of Mexico are located just to the southeast of the city. Although they are not included in this domain, the impact of these water bodies is introduced through the hourly boundary conditions obtained from the coarser meshes, and the intrusion of the Gulf breeze in Fig. 1 extends through most of the greater Houston area.

Time-height cross-sections of the potential temperature averaged over the 40x40 grid spaces within box B1 are shown in Fig. 2 for the three simulations. The general structure of the ABL evolution for all three runs is quite similar. The two simulations using the SGS closures (Fig. 2a,b) are nearly identical, indicating that the prognostic TKE closure and the Smagorinsky closure result in

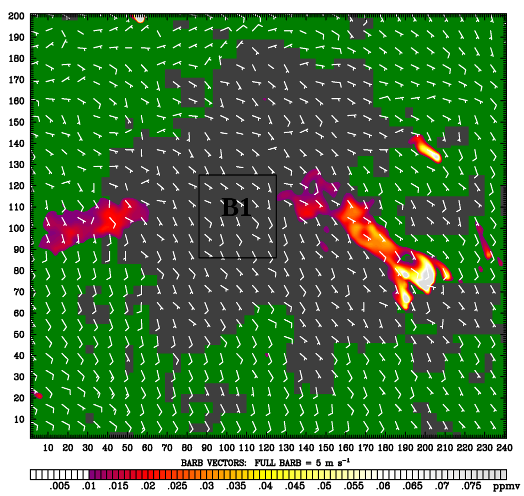

Fig. 1. Model domain for the 0.2km resolution simulations. Gray indicates urban landuse. Wind vectors and NO_x concentrations at 2200 UTC (5 pm local time) are also shown. The box (B1) indicates where averages were computed.

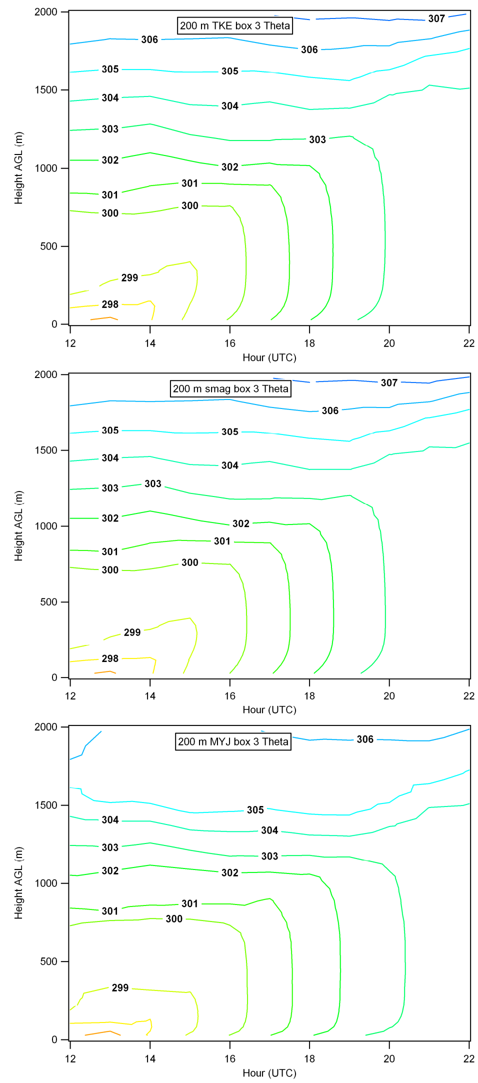

Fig 2. Time-height cross-sections of potential temperature averaged over Box B1, for simulations using the (a) TKE closure, (b) Smagorinsky closure, and (c) MYJ parameterization.

very similar vertical mixing. The simulation using the MYJ parameterization (Fig. 2c) shows an increasingly more super-adiabatic layer near the surface. In addition, the layer near the ABL top is slightly more stable. It appears that the two SGS schemes result in slightly stronger vertical mixing than the MYJ scheme.

Ozone concentrations at the lowest model level at the 5h forecast time (1700 UTC, noon local time) for the three simulations are shown in Fig. 3. In Houston, a cluster of emission point sources are located near the ship channel in the southeastern portion of the model domain (see Fig. 1). While ozone is not directly emitted, ozone precursors such as NO_x are in plentiful supply in this region. It is apparent that the two simulations using the SGS closures give very similar results in terms of ozone production and transport, while the simulation using the MYJ closure is noticeably different.

Fig 4 shows the ozone concentrations for the three model runs 4 hours later, at 2100 UTC (4pm local time). By this time, the sea breeze has penetrated to near the center of the domain. Again, the simulations with the SGS closures are similar, although differences between them are now noticeable. The simulation with the MYJ closure shows a somewhat different distribution of ozone, reflecting small differences in the low level advection and vertical mixing.

4. Conclusions

The two simulations with SGS closures produced a similar areal distribution of surface ozone concentrations. However, when vertical diffusion is determined by the MYJ parameterization, the simulated surface ozone concentrations are noticeably different. In addition, the parameterized boundary layer was slightly cooler and more super-adiabatic in the afternoon than the simulations with SGS closures.

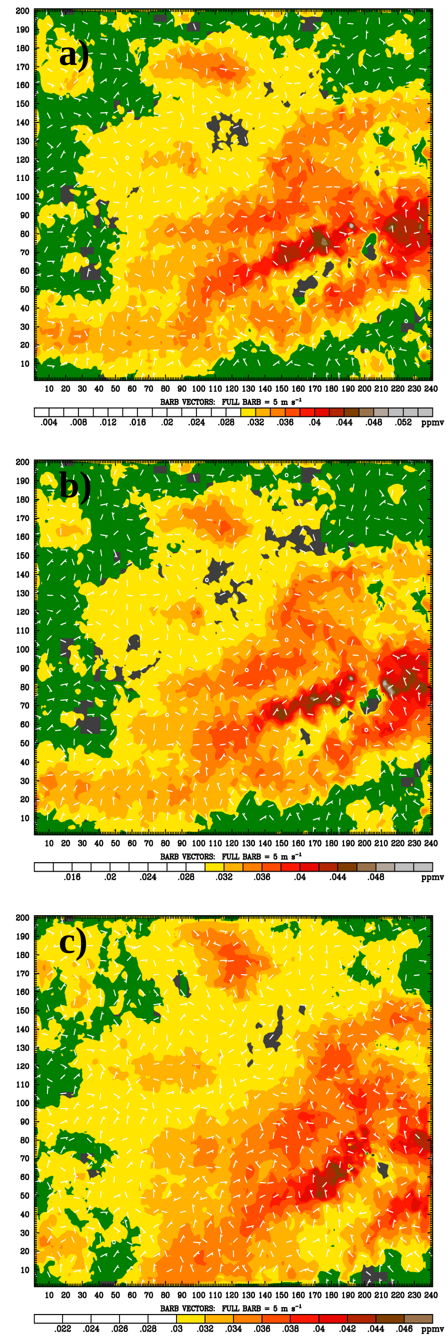

Fig 3. Ozone concentrations at the lowest model level at 1700 UTC (1200 local time) for a) the TKE closure, b) the Smagorinsky closure, and c) the MYJ parameterization.

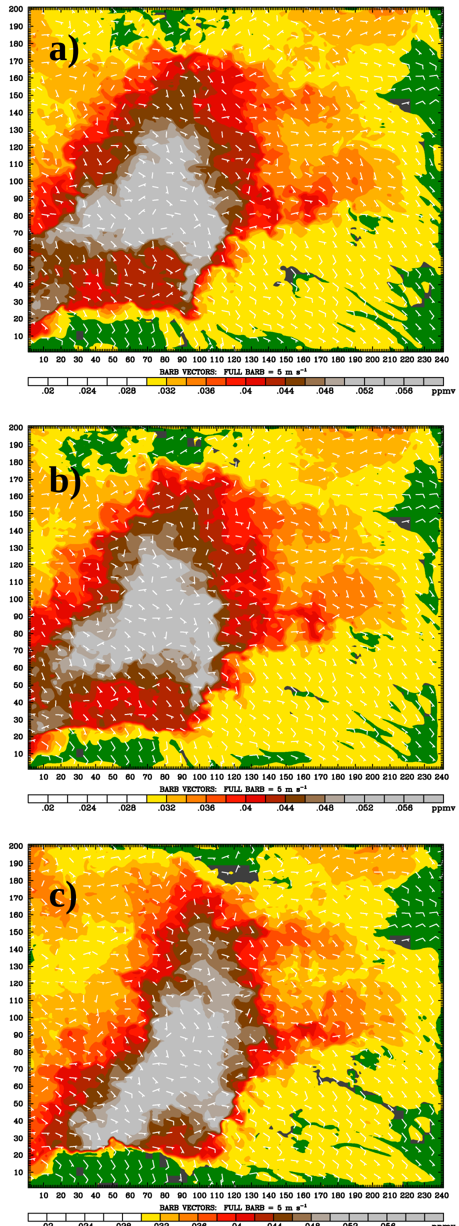

Fig 4. Ozone concentrations at the lowest model level at 2100 UTC (4pm local time) for a) the TKE closure, b) the Smagorinsky closure, and c) the MYJ PBL parameterization.

It would be premature to conclude that any one of the schemes is better than the others based on this single sensitivity study at 200m resolution. The fact that the simulations do not show a great sensitivity to the SGS closures indicates that vertical and horizontal advections, the resolvable part of the model solution, are the dominant flow components in this particular case.

The differences seen in these results, however, confirm the validity of the point made by Wyngaard (2004) that the conventional parameterization for sub-grid turbulence mixing in numerical weather prediction models may not be sufficient for the simulation of atmospheric boundary layer winds and temperature with grid spacing of 200 m. How to properly account for sub-grid turbulence mixing in fine-scale simulations still remains a challenge.

5. References

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