Atmospheric Boundary Layer Modeling for Combined Meteorology and Air Quality Systems

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Abstract Atmospheric Eulerian grid models for mesoscale and larger applications require sub-grid models for turbulent vertical exchange processes, particularly within the Planetary Boundary Layer (PBL). In combined meteorology and air quality modeling systems consistent PBL modeling of winds, temperature, humidity, and chemical concentrations is necessary for accurate simulation of chemical transport through the 3-d grid and accurate simulation of gas-phase and aerosol chemistry. A recently developed PBL model, known as the Asymmetric Convective Model version 2 (ACM2), has been designed to represent realistic turbulent transport of atmospheric constituents. The ACM2 has local and non-local components for transport in convective boundary layers. Evaluation of the ACM2 involves comparisons to observed vertical profiles of meteorology and chemistry. For example, simulations of the Weather Research and Forecast (WRF) model and the Community Multiscale Air Quality (CMAQ) model are compared to vertical profiles of potential temperature, water vapor mixing ratio, and several trace chemical species from aircraft and balloon soundings. The modeled vertical structures of chemical and meteorological parameters are consistent with observations.

1. Introduction

Parameterizations of the Planetary Boundary Layer (PBL) are important components in meteorology models and even more critical for air quality models where ground-level concentrations of pollutants are largely determined by the extent of vertical mixing. Thus, accurate and consistent simulation of the diurnal evolution and vertical mixing of meteorological and chemical species is essential for realistic simulation of these atmospheric variables. Simple closure for the turbulent flux terms of the Reynolds averaged equations, such as eddy diffusion, are reasonable when the scale of the turbulent motions is smaller than the vertical grid spacing of the model as is usually the case in stable or neutral conditions, but these assumptions break down in the convective boundary layer (CBL) where convective eddies often form in the atmospheric surface layer and rise through the entire depth of the CBL. Under such conditions, vertical fluxes can be counter to local gradients. To account for such large-scale transport, several models have been developed to include non-local components. Many of these models, which are commonly used in meteorology models, are based on gradient adjustments that are parameterized according to the surface heat flux. Thus, these models are most valid for modeling heat fluxes and are not easily adapted for chemical transport modeling. The Asymmetric Convective Model version 2 (ACM2) is a hybrid model that similarly combines local and non-local components for comprehensive treatment of all stability conditions. However, unlike the gradient adjustment schemes, the ACM2's non-local component is equally valid for any atmospheric quantity because it is a simple transilient matrix scheme that describes the mass flux exchange between non-adjacent grid layers. The basic formulation, 1-D testing against large eddy simulations and field experiments, and evaluation within a mesoscale meteorology model are described in detail by Pleim (2007a&b). This paper provides preliminary evaluation of combined meteorology and air quality modeling using the ACM2 in the Weather Research and Forecast (WRF) and Community Multiscale Air Qualilty (CMAQ) models based on field data from the Texas Air Quality Study 2 (TexAQS II).

2. Modeling

The Advance Research WRF (ARW) version 3 was run for the TexAQS II period (August 1 – October 15, 2006) with 12 km grid cell size and 34 vertical layers on a domain that covers the eastern 2/3 of the continental US. The WRF simulations include the Pleim-Xiu LSM and the ACM2, which are available in WRF version 3. Details of the model configuration and a comprehensive model evaluation are presented by Gilliam and Pleim (2009). The WRF model simulations were used to drive CMAQ modeling for the same period. Note that these air quality simulations are to be considered as preliminary because the emissions were based on the National Emissions Inventory without the more detailed inventory for Texas that has been prepared by the Texas Commission on Environmental Quality. To ensure consistency between meteorology and air chemistry, the CMAQ was configured to use the ACM2 for turbulent transport of chemical species and to use land surface parameters from the PX LSM for calculation of chemical dry deposition.

3. PBL heights

The TexAQS II field experiment included eleven radar wind profilers in East Texas during the study period. Reliable techniques have been developed to estimate the PBL height for daytime hours from the radar raw data (Bianco et al. 2008). These derived PBL height data have been paired in time at each profiler site with the PBL heights estimated by the ACM2 in the WRF model simulations.

Figure 1 shows modeled and observed values for four of these profilers. The lines represent the median values at each hour of the day for the simulation period (August 1 – October 15) and the bars indicate the 25% and 75% values for each model and observed distribution. For three out the four sites shown the model overpredicts the median PBL height by about 100-300 m for most of the day. The interquartile ranges, however, almost always overlap. It is not clear how much of these differences are due to model error and how much is due to differences in technique. For example, the late afternoon collapse of the model PBL heights that results in consistent overprediction is probably an artifact of the model's PBL height algorithm that is very sensitive to the near surface temperature and surface heat flux. The profiler PBL height algorithm, on the other hand, is more sensitive to indicators of ambient turbulent intensities. Thus, residual turbulence can lead to gradual declines in observed PBL height while the model algorithm senses the initial stabilization of the lowest layers resulting in very low PBL heights. It is conceivable that the mid-day overpredictions could have a similar algorithmic cause.

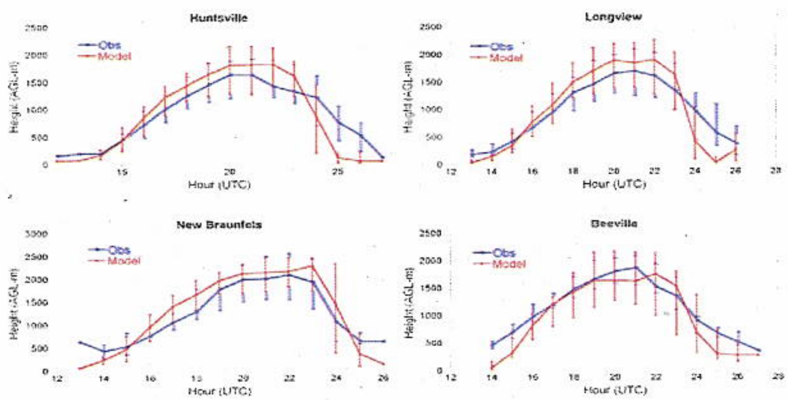

Fig. 1 Comparison of modeled and observed PBL height for August 1 – October 15, 2006

4. Aircraft Measurements

Aircraft measurements were important components of the TexAQS II experiment. The NOAA WP-3D Lockheed Orion aircraft (P3) made flights over east Texas region during Sept. 11 – Oct. 12, 2006. On several occasions the P3 flew a spiral flight path that extended well above the PBL. These sections of the flight measurements gave valuable evidence of the vertical structure of meteorological and chemical parameters within and above the PBL. Figure 2 shows an example of vertical profiles for potential temperature, water vapor mixing ratio, and NO_y for a P3 spiral about 120 km SE of Dallas at 19 UTC on 9/25/2006 compared to the model simulations from the WRF-CMAQ system. Although the NO_y concentration and water vapor mixing ratio are underpredicted in the PBL, the PBL structure is quite accurate for both meteorological and chemical parameters.

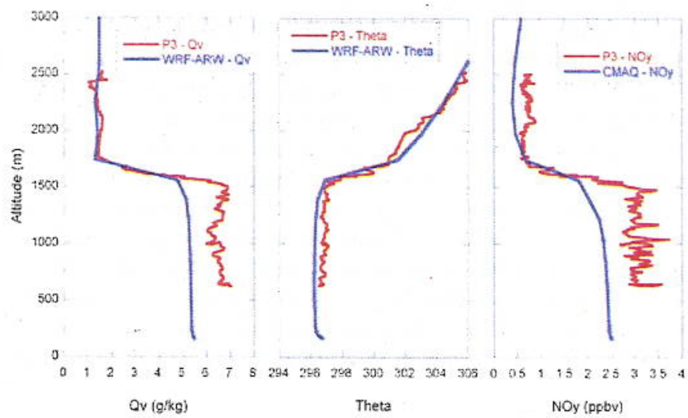

Figure 2. Modeled and observed profiles from P3 spiral at 19 UTC on 9/25/2006

5. Next steps

New CMAQ runs that include the special Texas emissions inventory and a 4 km horizontal nested grid domain centered on Houston are underway. Meteorology and chemistry model results will be compared to all of the P3 flight measurements with particular emphasis on the vertical spirals. Balloon data and aircraft lidar data will also be used to evaluate the vertical structure of meteorological and chemical fields.

Disclaimer: Although this paper has been reviewed by EPA and approved for publication, it does not necessarily reflect EPA's policies or views.

References

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