Atmospheric Environment 44 (2010) 523–532

Contents lists available at ScienceDirect

Atmospheric Environment

journal homepage: www.elsevier.com/locate/atmosenv

Improving ozone modeling in complex terrain at a fine grid resolution: Part I – examination of analysis nudging and all PBL schemes associated with LSMs in meteorological model

Yunhee Kim, Joshua S. Fu*, Terry L. Miller

Department of Civil & Environmental Engineering, University of Tennessee, Knoxville, TN 37996-2010, USA

ARTICLE INFO

Article history:
Received 27 April 2009
Received in revised form
17 September 2009
Accepted 29 October 2009

Keywords:
Model performance
CMAQ
Planetary boundary layer
Land surface model
Nudging analysis

ABSTRACT

Meteorological variables such as temperature, wind speed, wind directions, and Planetary Boundary Layer (PBL) heights have critical implications for air quality simulations. Sensitivity simulations with five different PBL schemes associated with three different Land Surface Models (LSMs) were conducted to examine the impact of meteorological variables on the predicted ozone concentrations using the Community Multiscale Air Quality (CMAQ) version 4.5 with local perspective. Additionally, the nudging analysis for winds was adopted with three different coefficients to improve the wind fields in the complex terrain at 4-km grid resolution. The simulations focus on complex terrain having valley and mountain areas at 4-km grid resolution. The ETA M–Y (Mellor–Yamada) and G–S (Gayno–Seaman) PBL schemes are identified as favorite options and promote O_3 formation causing the higher temperature, slower winds, and lower mixing height among sensitivity simulations in the area of study. It is found that PX (Pleim–Xiu) simulation does not always give optimal meteorological model performance. We also note that the PBL scheme plays a more important role in predicting daily maximum 8-h O_3 than land surface models. The results of nudging analysis for winds with three different increased coefficients' values (2.5, 4.5, and $6.0 \times 10^{-4}\ s^{-1}$) over seven sensitivity simulations show that the meteorological model performance was enhanced due to improved wind fields, indicating the FDDA nudging analysis can improve model performance considerably at 4-km grid resolution. Specifically, the sensitivity simulations with the coefficient value (6.0×10^{-4}) yielded more substantial improvements than with the other values (2.5 and 4.5×10^{-4}). Hence, choosing the nudging coefficient of $6.0 \times 10^{-4}\ s^{-1}$ for winds in MM5 may be the best choice to improve wind fields as an input, as well as, better model performance of CMAQ in the complex terrain area. As a result, a finer grid resolution is necessary to evaluate and access of CMAQ results for giving a detailed representation of meteorological and chemical processes in the regulatory modeling. A recommendation of optimal scheme options for simulating meteorological variables in the complex terrain area is made.

1. Introduction

The three-dimensional (3D) Air Quality Models (AQMs) for the State Implementation Plans (SIPs) of ozone (O_3) have been gaining increased attention because of playing an important role in guiding the development of regulatory modeling with the National Ambient Air Quality Standards (NAAQS) (Zhang et al., 2006). The non-attainment areas for the 8-h ozone designated by the U.S. Environmental Protection Agency (USEPA) must demonstrate the attainment using the 3D AQMs to see if the NAAQS for 8-h ozone does or does not meet a monitoring area of interest. Thus, each State having 8-h O_3 non-attainment areas are required to submit the SIPs to show for attainment of the 8-h NAAQS which currently meets less than 85 ppb at a localized monitoring area. Models generally tend to concentrate on how well models represent real values. However, there are many uncertainties in meteorological and photochemical models, and those responsibilities for decisions on control strategies need to use modeled scenarios without concern that inaccuracies and assumptions in the modeling may mislead them.

For the ozone SIPs modeling, air quality model performance at finer grid resolutions in the non-attainment areas is desirable because it is expected to propagate the actual structure of the atmosphere and show a more detailed representation of emissions, land-use, meteorological, and chemical processes as well as ozone control strategy. Thus, USEPA recommends that using 4 km

* Corresponding author. Tel.: +1 865 974 2629.
E-mail address: jsfu@utk.edu (J.S. Fu).

1352-2310/$ – see front matter Published by Elsevier Ltd.
doi:10.1016/j.atmosenv.2009.10.045

horizontal grid may be desirable for urban and fine scales of nested regional grids (EPA, 2007). However, recent studies have presented the impacts of grid resolutions such as 36-, 12-, and 4-km for the evaluation of model performance. According to Mathur et al. (2005), 4-km simulation provided the most accurate and realistic ozone prediction while Arunachalam et al. (2006), Cohan et al. (2006), Queen and Zhang (2008), and Wu et al. (2008) found that 4-km grid resolution did not always produce the better model performance of meteorology and CMAQ (Byun and Schere, 2006). As a result, the 12-km grid simulation became more widely and properly chosen. In addition, for the Visibility Improvement State and Tribal Association of the Southeast (VISTAS)'s regional problem in the Southeast US was addressed by conducting the meteorological modeling at 36- and 12-km. Consequently, the PX PBL produced credible meteorological variables (VISTAS, 2004). As a result, the PX model was the preferred choice to provide meteorological inputs to AQMs. However, as indicated by Cohan et al. (2006), the results obtained from finer grid resolutions become necessary when localized variability is needed. Hence, sensitivity simulations from finer grid resolutions for ozone non-attainment areas would be necessary. This is critically important when CMAQ assessment and evaluation are performed in the regulatory modeling.

There are schemes and nudging analyses that may perform differently. Newtonian relaxation or nudging analysis is one method of four-dimensional data assimilation (FDDA). The nudging method described by Stauffer et al. (1991) and Stauffer and Seaman (1994) was found to be an effective and economical method for performing FDDA. In particular, some studies have shown that using nudging analysis in MM5 is considered valuable because it can provide improved wind fields (Bao and Errico, 1997; Barna and Lamb, 2000; Cohan et al., 2006). At the fine scale, selecting the appropriate nudging coefficients may have impacts on MM5 and CMAQ simulation. The magnitude of the impact of nudging coefficients in MM5 on the CMAQ simulations has not been quantified at a fine grid resolution. Determining the appropriate value of nudging in MM5 to the CMAQ simulation can be useful to improve model performance at a finer grid resolution for SIPs in the non-attainment areas. When nudging is used in MM5 to create inputs for CMAQ, it is expected that the improvements of wind fields, shown in MM5 with nudging, would also improve daily maximum 8-h ozone concentration in the CMAQ simulation.

The PBL height in meteorological models plays an important role for predicting and understanding ozone formation and other pollutants (Perez et al., 2006). The PBL has a thickness ranging from a hundred meters to a few kilometers and affects the dynamical and thermal forcing at the surface. Pollutants are emitted into the mixing layer (ML) and become gradually dispersed and mixed through the action of turbulence under convective (Seibert et al., 2000). Hence, the various PBL schemes in MM5 are needed to account for the influence of PBL or ML on ozone air quality during the typical ozone summer season in the complex terrain. CMAQ is then executed by forcing meteorological conditions as an input produced by a single configuration of MM5 (Mao et al., 2006). Some studies have shown how various PBL schemes affect the concentration of pollutants of CMAQ. Still, there is a lack of evaluation concerning how PBL schemes associated with LSMs affect CMAQ model performance at 4-km grid resolution.

The primary objective of this paper is to evaluate the performance of the meteorological model and CMAQ in the complex terrain at a 4-km grid resolution for ozone SIPs. We will also examine the impacts of nudging analysis for winds (and various PBL schemes associated with LSMs in MM5 on CMAQ simulation), to identify the most appropriate PBL schemes associated with LSMs and to determine the best nudging coefficient value for winds. We will present our results in two parts. Part I describes the influence of various nudging coefficients for winds, and five different PBL schemes associated with three different LSMs (21 sensitivity simulation scenarios) on meteorological fields at 4-km horizontal grid resolution to provide a better representation of the meteorology. It also presents impacts of meteorological fields on grid size resolutions of 12-km and 4-km with the PX PBL scheme. Part II focuses on daily maximum 8-h ozone concentrations from the 21 sensitivity simulation scenarios results of CMAQ.

Overall, the results of the study will provide a recommendation of the MM5 and CMAQ configurations for ozone SIP modeling exercises in the complex terrain areas. In addition, this study might provide thoughtful implications for giving a right decision that helps to improve the air quality management and their impacts on ozone SIPs to the State having 8-h O_3 non-attainment areas.

2. Methodology

2.1. Modeling components

The MM5–MCIP–SMOKE–CMAQ modeling system was used in this study. Version 3.7 of MM5 was used to generate meteorological fields for CMAQ as inputs. The output from MM5 was processed by MCIP (Meteorology Chemistry Interface Processor) version 3.1 (Byun and Ching, 1999). It was used and needed by SMOKE Version 2.1 (Houyoux et al., 2002) and CMAQ Version 4.5 as a proper format.

2.2. Episode selection

The 31-day episode was selected for the simulation to represent the typical summer condition. The summer episode is from 1 August to 31 August for the year of 2002 and included a 5-day spin-up period starting at 26 July 2002. The month of August was chosen for the simulation due to the fact that the model performance of the month of August showed generally poor conditions.

2.3. Description of the meteorological modeling

MM5 is a non-hydrostatic, prognostic, and mesoscale meteorological model developed by the Fifth Generation Pennsylvania State University, National Center for Atmospheric Research (Dudhia et al., 2004). The 4 km modeling domain covers East Tennessee, and a portion of several surrounding states including North Carolina (NC), South Carolina (SC), Georgia (GA), West Virginia (WV), and Alabama (AL). Fig. 1 and Table 1 show the Visibility Improvement State and Tribal Association of the Southeast (VISTAS)'s 36 km and 12 km domains, the nested 4 km domains, and all seven monitoring sites representing valley sites (Anderson, Mildred, Rutledge, and Jefferson) and for mountain sites (Look Rock, Cove Mt., and Clingman's Dome) observed in this study. The nested 4 km domain extracted VISTAS's 12 km outputs as its boundary and initial condition inputs. The 36 and 12 km model domains had 34 layers, performed with PX PBL scheme, Kain-Fritsch2 (KF2) cloud scheme, RRTM radiation scheme, and mixed-phase microphysics scheme in the current VISTAS's model configuration.

The INTERPPX is a new preprocessor used to initialize soil moisture, temperature, and canopy moisture from a previous run after NESTDOWN (Pleim and Chang, 1992). This method is only applied for PX model. The NESTDOWN is used to generate inputs for finer grid resolution MM5 run from the coarser resolution MM5 output. One-way NESTDOWN method was selected to generate inputs for the 4-km grid resolution MM5 run. This took output from MM5 run, together with TERRAIN output for a 4-km grid domain.

The 4-km grid resolution has 127 by 118 grids with 34 layers in MM5. The MM5 model was in Lambert conformal projection with true latitudes at 33° N and 45° N. The 4-km grid domain also