Particuology xxx (2018) xxx–xxx

Contents lists available at ScienceDirect

Particuology

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

Comparative evaluation of the impact of GRAPES and MM5 meteorology on CMAQ prediction over Pearl River Delta, China

Tao Deng[a,*], Yiang Chen[a,b], Qilin Wan[a], Yanxia Zhang[a], Xuejiao Deng[a], Yanyan Huang[a], Guangfeng Dai[a], Fei Li[a]

[a] *Institute of Tropical and Marine Meteorology/Guangdong Provincial Key Laboratory of Regional Numerical Weather Prediction, China Meteorological Administration, Guangzhou 510080, China*

[b] *Key Laboratory of Meteorological Disaster, Ministry of Education, Joint International Research Laboratory of Climate and Environment Change, Collaborative Innovation Center on Forecast and Evaluation of Meteorological Disasters, Key Laboratory for Aerosol-Cloud-Precipitation of China Meteorological Administration, Nanjing University of Information Science & Technology, Nanjing 210044, China*

ARTICLE INFO

Article history:
Received 26 March 2017
Received in revised form 8 October 2017
Accepted 13 October 2017
Available online xxx

Keywords:
Air quality
Numerical simulation
Global/regional assimilation and prediction system (GRAPES)
Community multiscale air quality (CMAQ)
Process analysis

ABSTRACT

The community multiscale air quality (CMAQ) model was used to forecast air quality over the Pearl River Delta region from December 2013 to January 2014. The pollution forecasting performance of CMAQ coupled with two different meteorological models, i.e., the global/regional assimilation and prediction system (GRAPES) and the fifth-generation mesoscale model (MM5), was assessed by comparison with observational data. The effects of meteorological factors and physicochemical processes on the forecast results were discussed through process analysis. The results showed that both models exhibited good performance but that of GRAPES-CMAQ was better. GRAPES was superior in predicting the overall variation tendencies of meteorological fields, but it showed large deviations in atmospheric pressure and wind speed. This contributed to the higher correlation coefficients of the pollutants with GRAPES-CMAQ but with greater deviations. The underestimations of nitrate and ammonium salt contributed to the underestimations of both particulate matter and extinction coefficients. Source emissions made the only positive contributions to surface layer SO_2, CO, and NO. It was found that O_3 originated primarily from horizontal and vertical transport and that its consumption was predominantly via chemical processes. Conversely, NO_2 was found derived primarily from chemical production.

Introduction

The Pearl River Delta (PRD) region, which ranks highly among those regions of China that have recently experienced rapid economic development, is beset with severe environmental problems. Its special geographical position with surrounding mountains on three sides contributes to the accumulation of emitted airborne pollutants. These can interact to form regional compound-type atmospheric pollution, especially in autumn and winter, which reduces visibility and causes frequent hazy weather (Chan & Yao, 2008; Deng et al., 2008; Hagler et al., 2006; Wu et al., 2005). Following concerted atmospheric environmental research and the rapid development of computing technology, numerical models used for simulations of air quality have developed from simple Gaussian models to complex multiscale three-dimensional numerical forecasting systems. Thus, numerical modeling has been adopted by the research community as one of primary methods for studying air pollution (Grell et al., 2005; Jiang et al., 2010; Morris et al., 2006; Tie, Geng, Peng, Gao, & Zhao, 2009; Wang, Carmichael, Chen, Tang, & Wang, 2005; Wang, Guo, Jiang, Ling, & Wang, 2015; Wu et al., 2014). In particular, constant improvement in emission inventory precision (Lu et al., 2013; Streets & Waldhoff, 2000; Zhang et al., 2009; Zhang, Geng, Wang, Richter, & He, 2012; Zheng, Zheng, Wang, Zhong, & Wu, 2009) has provided a basis for regional air quality numerical forecast operations. The PRD air quality numerical forecasting system has been in operation since 2009 (Deng, Deng et al., 2012; Deng et al., 2013). Application of both source assimilation (Cheng, Xu, & Ding, 2010; Xu et al., 2008; Yumimoto, Uno, Sugimoto, Shimizu, & Satake, 2007) and initial field assimilation (Denby, Schaap, Segers, Builtjes, & Horálek, 2008; Jiang et al., 2013; Liu, Liu et al., 2011; Pagowski & Grell, 2012; Wu, Mallet, Bocquet,

---

* Corresponding author.
E-mail address: tdeng@grmc.gov.cn (T. Deng).

https://doi.org/10.1016/j.partic.2017.10.005
1674-2001/© 2018 Chinese Society of Particuology and Institute of Process Engineering, Chinese Academy of Sciences. Published by Elsevier B.V. All rights reserved.

Please cite this article in press as: Deng, T., et al. Comparative evaluation of the impact of GRAPES and MM5 meteorology on CMAQ prediction over Pearl River Delta, China. *Particuology* (2018), https://doi.org/10.1016/j.partic.2017.10.005

& Sportisse, 2008) has improved considerably the simulation capability for specific pollutants.

The precision of an air quality model depends largely on the accuracy of the forecasts of various meteorological fields (Meij et al., 2009; Smyth et al., 2006; Venkatram, 2004). Appel, Roselle, Gilliam, and Pleim (2010) compared the operational performances of two community multiscale air quality (CMAQ) model simulations that used input data from the fifth-generation mesoscale model (MM5) and the weather research and forecasting (WRF) meteorological model. They found WRF-CMAQ was superior to MM5-CMAQ in simulating sulfate and nitrate but slightly inferior in simulating black carbon (BC). Based on comparative evaluation of the impact of WRF-NMM (Nonhydrostatic Mesoscale Model) and WRF-ARW (Advanced Research WRF) meteorology on CMAQ simulations of $PM_{2.5}$, its related precursors, and O_3, Yu et al. (2012a, 2012b) from overestimations of SO_4^{2-}, NO_3^-, and NH_4^+, and greater underestimation of $PM_{2.5}$ in suburban areas by NMM-CMAQ resulted from underestimations of SO_4^{2-}, OC, and EC. Of the two models, ARW-CMAQ had slightly better performance for O_3. Fan et al. (2013) assessed the simulation performance of CMAQ driven by three meteorological fields. They found that the correlation coefficients were best with MM5 and that the simulated SO_2 root-mean-square error was minimum with WRF incorporating four-dimensional data assimilation (WRF/FDDA). Wong et al. (2011) succeeded in decreasing considerably the simulation biases of surface shortwave radiation and 2-m temperature, and they improved the forecasting performance for $PM_{2.5}$ and O_3 using an online WRF-CMAQ (two-way coupled system with aerosol feedback) with consideration of the direct radiation feedback of aerosols. Research on the air quality of the PRD region by Deng, Wu et al. (2012) using MM5-CMAQ showed that haze events were caused primarily by secondary aerosols, and that the extinction contribution rate of secondary aerosols exceeded 70% when relative humidity was >90%.

This study had a number of objectives based on numerical forecasting simulations for the PRD region in winter using CMAQ: (1) to compare the global/regional assimilation and prediction system (GRAPES)- and MM5-driven forecast results of pollutant concentrations, (2) to analyze the pollution forecasting performance of CMAQ coupled with different meteorological models, (3) to analyze pollutant production and transport mechanisms by combining CMAQ with process analysis (PA), (4) to assess the principal forecasting error sources, and (5) to compare pollutant formation and transport effects among different cities within the PRD region.

Methods and data

Model introduction

The air quality model system adopted in this study comprised the GRAPES/MM5, sparse matrix operator kernel emissions (SMOKE), and CMAQ models.

GRAPES is a new-generation, nonhydrostatic, multiscale universal numerical forecasting model developed independently in China, and it serves as a unified model targeted at weather and climate and adaptable both regionally and globally. This model uses a semi-implicit, semi-Lagrangian time integral scheme, an Arakawa C-grid for longitude–latitude grid point design, a Charney–Philips vertical staggered arrangement, and height-based terrain-following coordinates. The main physical components include an explicit grid-scale cloud precipitation formulation scheme, subgrid-scale cumulus convection scheme and radiation scheme, as well as heat and momentum, vertical transport of water vapor and hydrometeors, and boundary layer and land surface processes (Chen et al., 2008; Zhong & Chen, 2015). In this study, GRAPES was used for various physical schemes including the WRF single-moment 6-class (WSM6) microphysical scheme, the rapid radiative transfer model (RRTM) longwave radiation scheme, the European Centre for Medium-Range Weather Forecasts (ECMWF) shortwave radiation scheme, the surface layer Monin–Obukhov (M–O) similarity theory, the medium range forecast (MRF) boundary layer scheme, the SLAB land surface process scheme, and the simplified Arakawa–Schubert (SAS) cumulus convection scheme. The cycle of hourly assimilation and forecast system (CHAF), developed by the Guangzhou Institute of Tropical and Marine Meteorology of the China Meteorological Administration, was employed to assimilate air sounding, ground surface, ship, and radar data (Huang, Wan, Chen, Zhang, & Ding, 2011).

MM5, referring to the mesoscale model developed jointly by the University of Pennsylvania (USA) and National Center for Atmospheric Research (NCAR), is a widely used simulation system involving modules for terrain data processing, surface data processing, air sounding data processing, objective analysis, initialization, numerical forecasting, and postprocessing. It is capable of achieving multiple nesting and easy positioning for different geographic locations (Grell, Dudhia, & Stauffer, 1994). Here, MM5 version 3.7 was used, which included the mixed-phase microphysical scheme, Grell cumulus cloud scheme, MRF boundary layer scheme, RRTM longwave radiation scheme, and Noah land surface process scheme.

SMOKE is a state-of-the-art emission inventory processing system (Houyoux, Vukovich, Brandmeyer, Seppanen, & Holland, 2004) that has been developed and improved by the University of North Carolina (USA). It is used primarily for processing emission inventory data into input data for atmospheric chemistry models. It is capable of determining spatiotemporal distributions and chemical species of emission inventories and calculating hourly emissions of natural sources and mobile sources. SMOKE version 2.4 was adopted in this study. Its emission source was the PRD atmospheric emission inventory using 2006 as the base year and using the Asian emission inventory (INTEX-B2006) as the background. The emission data of INTEX-B2006 were treated with a spatial interpolation method to fit the model domain. The PRD atmospheric emission inventory was updated to 2009 (Zheng et al., 2009) with 3-km resolution, and reproductive distribution was performed on surface source spatial distributions based on satellite-derived data (Liu et al., 2016). The temporal resolution of the original emission data was yearly. Here, the temporal allocation of the dataset followed Zheng et al. (2009), and the final resolution was converted to hourly by SMOKE.

The CMAQ model refers to a multiscale atmospheric photochemistry mass model developed by the U.S. Environmental Protection Agency. It represents the latest mainstream research achievements on atmospheric chemistry, pollutant transfer, and deposition. It is capable of simulating relocation diffusion and chemical reactions of multiple atmospheric pollutants such as O_3, aerosols, and acid deposition (Byun & Schere, 2006). CMAQ version 5.0.1 was adopted in this study. It incorporated the gaseous-phase and aerosol mechanism cb05_ae5_aq, and it considered the influences of aqueous-phase chemistry, water phase/cloud processes, and sea salt. The sea salt was calculated online by CMAQ, whereby oceanic sea salt emissions were calculated based on wind speed and relative humidity (Gong, 2003; Zhang, Knipping, Wexler, Bhave, & Tonnesen, 2005). Visibility is related to an extinction coefficient. Extinction coefficients, determined by the extinction characteristics of aerosols, are strongly associated with aerosol composition and relative humidity. Here, the extinction effect for various aerosol components was subjected to parametric calculation (Malm, Sisler, Huffman, Eldred, & Cahill, 1994; Sisler & Malm, 1994).

The meteorological model used National Centers for Environmental Prediction (NCEP) global forecast system (GFS) data with resolution of 0.25° as the boundary and initial fields, and global NCEP 30 s terrain data and 30 s United States Geological Sur-

Please cite this article in press as: Deng, T., et al. Comparative evaluation of the impact of GRAPES and MM5 meteorology on CMAQ prediction over Pearl River Delta, China. *Particuology* (2018), https://doi.org/10.1016/j.partic.2017.10.005