Particuology 20 (2015) 41–51

Contents lists available at ScienceDirect

Particuology

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

Modeling study of a severe aerosol pollution event in December 2013 over Shanghai China: An application of chemical data assimilation

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ARTICLE INFO

Article history:
Received 29 July 2014
Received in revised form 16 October 2014
Accepted 21 October 2014

Keywords:
Data assimilation
Aerosol pollution
Initial condition
Forecasting
$PM_{2.5}$

ABSTRACT

This study focuses on the importance of initial conditions to air-quality predictions. We ran assimilation experiments using the WRF-Chem model and grid-point statistical interpolation (GSI), for a 9-day severe particulate matter pollution event that occurred in Shanghai in December 2013. In this application, GSI used a three-dimensional variational approach to assimilate ground-based $PM_{2.5}$ observations into the chemical model, to obtain initial fields for the aerosol species. In our results, data assimilation significantly reduced the errors when compared to a simulation without assimilation, and improved forecasts of $PM_{2.5}$ concentrations. Despite a drop in skill directly after the assimilation, a positive effect was present in forecasts for at least 12–24 h, and there was a slight improvement in the 48-h forecasts. In addition to performing well in Shanghai, the verification statistics for this assimilation experiment are encouraging for most of the surface stations in China.

Introduction

Chemical forecasting is challenging primarily because of large uncertainties related to boundary/initial conditions, physical/chemical processes, and emission sources (Alapaty, Olerud, Schere, & Hanna, 1995; Barna & Knipping, 2006; Biswas & Rao, 2001; Hanna et al., 2001; Guenther, Zimmerman, Harley, Monson, & Fall, 1993; Lee et al., 2008; Mathur, Schere, & Nathan, 1994; Sillman & Samson, 1995; Zhang & Rao, 1999). The aim of data assimilation is to integrate observations into forecasts. Major meteorological centers have traditionally applied data assimilation to provide optimal initial conditions for numerical weather models (Gauthier, Tanguay, Laroche, Pellerin, & Morneau, 2007; Lorenc et al., 2000; Parrish & Derber, 1992;Rabier, Järvinen, Klinker, Mahfouf, & Simmons, 2000). However, chemical data assimilation has not been equally well developed, and is not commonly applied. Many operational air-quality models are initialized using concentrations of chemical species obtained from the previous day's forecast, without considering observations. Data assimilation has not been extensively applied to air-quality models because chemical observations are relatively scarce compared to meteorological observations, especially with respect to vertical profiles. Recent progress in chemical models and ground-based monitoring networks has aided the development and implementation of aerosol data assimilation. Data assimilation in chemical models improves initial conditions and provides tools for better estimates of emission intensity. The main assimilation methods applied to chemical models include three-dimensional variational (3D-Var), four-dimensional variational (4D-Var), and ensemble Kalman filters.

Elbern et al. (Elbern, Schmidt, & Ebel, 1997; Elbern, Schmidt, Talagrand, & Ebel, 2000; Elbern & Schmidt, 1999, Elbern & Schmidt, 2001) developed a 4D-Var assimilation model. Their results showed that the optimized emission factors significantly improved SO_2 forecasts and moderately improved O_3 forecasts. The initial conditions were a major factor in these improvements. Emissions had a smaller effect, which was possibly because of inadequate model resolution, chemical mechanism biases, and the coarse NO_x observation network.

The ensemble Kalman filter (EnKF) was introduced by Evensen (1994). EnKF applications for air quality modeling were studied by Chai et al. (2007), Constantinescu, Chai, Sandu, and

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http://dx.doi.org/10.1016/j.partic.2014.10.008

Carmichael (2007a), Constantinescu, Sandu, Chai, and Carmichael (2007b), Constantinescu, Sandu, Chai, and Carmichael (2007c), Constantinescu, Sandu, Chai, and Carmichael (2007d), Daescu and Carmichael (2003), Sandu, Daescu, Carmichael, and Chai (2005), Tang, Zhu, Wang, and Gbaguidi, 2011, and Tang et al., 2013. Different applications of EnKF to idealized and real data cases showed that this assimilation approach is promising, but methods of covariance inflation and localization that were essential for filter performance required further investigation. Even though there were improvements in the forecasting skill, no conclusion could be drawn on the relative importance of the initial conditions or emission and lateral boundary condition adjustments.

In this study, we applied a 3D-Var system, which includes the weather research and forecasting-chemistry model (WRF-Chem; Grell et al., 2005) and grid-point statistical interpolation (GSI). We used this system to assess the impact of surface fine aerosol ($PM_{2.5}$) measurement assimilations on the forecast skill. The feasibility and usefulness of the GSI assimilation algorithm were investigated in several papers (Li et al., 2013; Pagowski, Grell, McKeen, Peckham, & Devenyi (2010); Pagowski et al., 2014; Purser, Wu, Parrish, & Roberts, 2003a; Purser, Wu, Parrish, & Roberts, 2003b; Schwartz, Liu, Lin, & McKeen, 2012; Wu, Purser, & Parrish, 2002). Pagowski et al. (2010) assimilated surface $PM_{2.5}$ observations over the United States using GSI and noted improved aerosol forecasts. Here, we applied a similar approach to aerosol forecasts in China. We show that a simple chemical data assimilation of fine particulate matter improved the skill of chemical model forecasts for a highly polluted case in China. This improvement can be attributed to improved initial conditions, and only slightly increased the computational time.

In Data and model configuration section, we describe the ground-based measurement network and model configurations, including the modeling system and data assimilation method. Our results and discussions are presented in Result and discussion section, and our conclusions are given in Conclusion section.

Data and model configurations

In-situ measurements

Surface $PM_{2.5}$ concentrations over China are recorded by the monitoring network maintained by the Ministry of Environmental Protection. The monitoring network provides hourly-averaged PM_{10}, $PM_{2.5}$, O_3, NO_2, SO_2, and CO concentrations. We only considered $PM_{2.5}$ assimilation in this study. $PM_{2.5}$ measurements are readily available at all times with minimal delay, and can be used in real time for data assimilation or model evaluation. A map of the stations that measure $PM_{2.5}$ is shown in Fig. 1(a). There are approximately 315 sites within the model domain, and most are situated in low-lying areas. The stations are most densely distributed in three advanced economic regions: the Yangtze River Delta (YRD) in the east; the Beijing-Tianjin-Hebei Band (BTH) in the north; and Pearl River Delta (PRD) in the south of China. The next densest region is the eastern part of China (Fig. 1(a)). Measuring sites are relatively sparse in the middle and west of China. $PM_{2.5}$ observation sites are mostly located in urban and suburban areas. According to the spatial distribution of anthropogenic $PM_{2.5}$ emissions displayed in Fig. 1(b), most stations are located in the polluted area.

Model set-up

We ran numerical simulations using the WRF-Chem model, version 3.4.1. The WRF model is non-hydrostatic. The chemistry model is fully coupled with the WRF model, having the same vertical and horizontal coordinates, time steps, transport scheme, and physical parameterization schemes. A detailed description of WRF-Chem was given by Grell et al. (2005), and more information can be found on the WRF website (http://ruc.noaa.gov/wrf/WG11/).

The domain used in this study had 90 × 125 grid points, with a horizontal resolution of 27 km (Fig. 1(b)). The model has 35 vertical

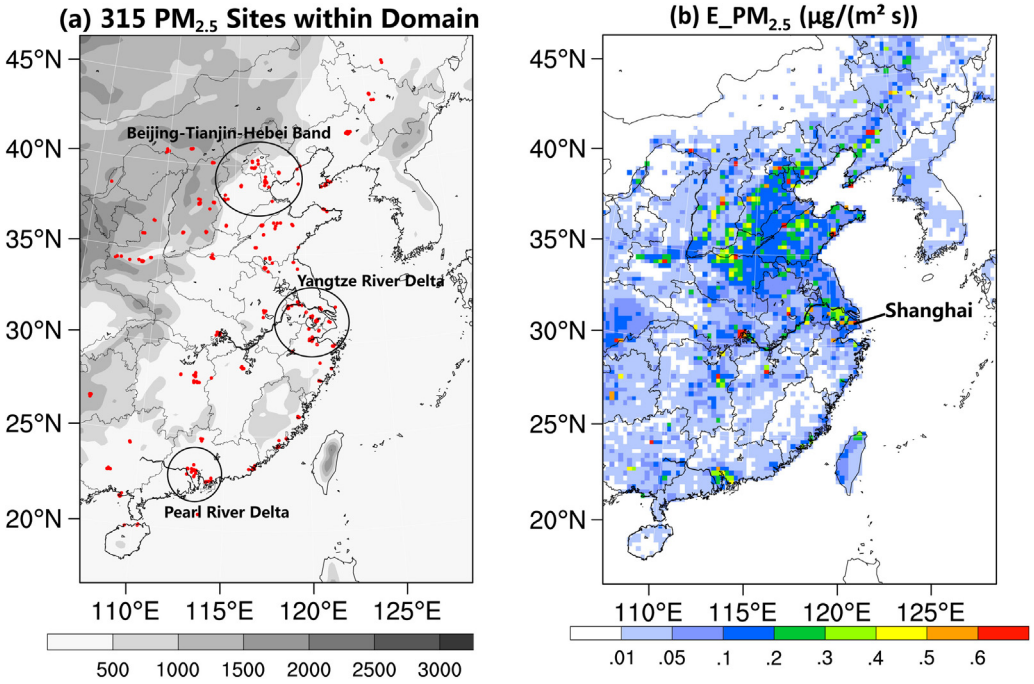

Fig. 1. Modeling domain with: (a) 315 $PM_{2.5}$ measurement sites (red points) and surface topography (shaded, m), and (b) anthropogenic emissions of E_$PM_{2.5}$ (μg/(m² s)). The three circles in (a) denote three advanced economic regions. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)