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Short communication

Persistence of initial conditions in continental scale air quality simulations

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HIGHLIGHTS

- Spin-up periods of ten days may not be sufficient for continental scale modeling.
- Initial conditions derived from global models may shorten required spin-up periods.
- Bi-directional modeling needs to consider the effects of soil initialization.

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ABSTRACT

This study investigates the effect of initial conditions (IC) for pollutant concentrations in the atmosphere and soil on simulated air quality for two continental-scale Community Multiscale Air Quality (CMAQ) model applications. One of these applications was performed for springtime and the second for summertime. Results show that a spin-up period of ten days commonly used in regional-scale applications may not be sufficient to reduce the effects of initial conditions to less than 1% of seasonally-averaged surface ozone concentrations everywhere while 20 days were found to be sufficient for the entire domain for the spring case and almost the entire domain for the summer case. For the summer case, differences were found to persist longer aloft due to circulation of air masses and even a spin-up period of 30 days was not sufficient to reduce the effects of ICs to less than 1% of seasonally-averaged layer 34 ozone concentrations over the southwestern portion of the modeling domain. Analysis of the effect of soil initial conditions for the CMAQ bidirectional NH_3 exchange model shows that during springtime they can have an important effect on simulated inorganic aerosols concentrations for time periods of one month or longer. The effects are less pronounced during other seasons. The results, while specific to the modeling domain and time periods simulated here, suggest that modeling protocols need to be scrutinized for a given application and that it cannot be assumed that commonly-used spin-up periods are necessarily sufficient to reduce the effects of initial conditions on model results to an acceptable level. What constitutes an acceptable level of difference cannot be generalized and will depend on the particular application, time period and species of interest. Moreover, as the application of air quality models is being expanded to cover larger geographical domains and as these models are increasingly being coupled with other modeling systems to better represent air-surface-water exchanges, the effects of model initialization in such applications needs to be studied in future work.

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1. Introduction

Eulerian air quality modeling systems used in research, forecasting, and air quality planning applications simulate atmospheric pollutant concentrations through the numerical representation of emissions, transport, transformation, and removal processes affecting pollutant concentrations. These models require the specification of initial and lateral boundary conditions. Ideally, these initial and boundary conditions would be based on observations, but in reality, this is not feasible due to the large number of species and extensive spatial domains handled by these models. Therefore, initial concentrations are often based on estimated climatological conditions (Byun and Schere, 2006) or global scale models while lateral boundary conditions often are derived from global scale models (Schere et al., 2012). Studying the effect of

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boundary conditions on regional air quality simulations continues to be a topic of active research interest due to the need to properly quantify large-scale background concentrations and intercontinental transport in regional applications (e.g. Schere et al., 2012; Dolwick et al., 2015; Giordano et al., 2015). On the other hand, little recent work has been performed to quantify the impact of initial conditions on simulated concentrations. While it is a generally accepted practice to "spin up" a model for a certain time period prior to the study period of interest to reduce or eliminate the effects of initial conditions, to our best knowledge no recent studies have been performed to quantify the necessary time periods for continental-scale applications. In the earlier days of regional air quality modeling, Brost (1988) performed sensitivity simulations with the Regional Acid Deposition Model (RADM) (Chang et al., 1987) and found that the effects of initial conditions on key reactive species became insignificant after a 2–3 day spin-up period for a domain covering 2400 by 2400 km. Berge et al. (2001) performed simulations with both a box model and regional air quality model for a domain over the San Joaquin Valley and found that, within the planetary boundary layer, the impact of initial conditions falls to < 10% after 48 h with the exception of PAN and HNO_3 at some locations. For the free troposphere, they found that impacts >10% were seen for reservoir species even after three days spin-up over larger portions of the domain. Over the following decade, a number of regional scale air quality applications used a spin-up period of three days (Sistla et al., 2001; Tao et al., 2003; Hogrefe et al., 2004; Foley et al., 2010). With the increasing number of model applications encompassing the entire conterminous U.S., spin-up periods were extended to ten days (Appel et al., 2010, 2012; Hogrefe et al., 2015); however, no formal analysis was presented in these studies to demonstrate that the increased spin-up period was sufficient to eliminate the effects of initial conditions.

In addition to applications at increasingly large domains, air quality modeling systems have also become more complex, integrating more interactions between the atmosphere and land surface, in part through coupling with other models. One example is the treatment of bidirectional NH_3 air/surface exchange implemented in the Community Multiscale Air Quality (CMAQ) model (Byun and Schere, 2006) as described in Bash et al. (2010, 2013) and Pleim et al. (2013). By including such interactions, the question of how model initialization affects simulated concentrations potentially needs to be expanded beyond the traditional focus on atmospheric initial conditions to include initial conditions in other media such as concentrations in the soil. The present study addresses both the persistence of atmospheric initial conditions for continental-scale applications and the persistence of soil initial condition effects in CMAQ applications using the bidirectional NH_3 flux approach.

2. Model simulations

The regional air quality simulations analyzed in this study were performed with version 5.0.2 of CMAQ. Meteorological fields were prepared using version 3.4 of the Weather Research and Forecasting (WRF) model (Skamarock and Klemp, 2007). Throughout the WRF simulation, nudging of temperature, wind speed, and water vapor mixing ratio was applied above the PBL following the approach described in Gilliam et al. (2012). In addition, soil temperature and moisture nudging as described in Pleim and Xiu (2003) and Pleim and Gilliam (2009) was applied as well. The 2010 emission inputs are described in Pouliot et al. (2015). The CMAQ simulations were performed with a horizontal grid spacing of 12 km over the continental U.S. with a vertical extent to 50 mb (roughly 20 km above sea level) using 35 vertical layers. Model layer 34 used in some of the analyses presented in Section 3 extends roughly from 13.8 km to 16.2 km above sea level. Chemical boundary conditions were prepared from global concentration fields simulated by the European Center for Medium Range Weather Forecasts (ECMWF) Composition – Integrated Forecast System (C-IFS) model (Flemming et al., 2015). Additional details on the configuration of WRF and CMAQ can be found in Solazzo et al. (2017). Four sets of simulations were performed to study the effects of initial conditions on simulated air quality. The first simulation, serving as reference simulation and hereafter referred to as BASE, was initialized on December 22, 2009 and run continuously to August 31, 2010. The second simulation, hereafter referred to as SPRING_PROF, was initialized on February 23, 2010 and run to April 30, 2010. The third and fourth simulations, hereafter referred to as SUMMER_PROF and SUMMER_CIFS, were initialized on June 21, 2010 and run to August 31, 2010. By contrasting the results from the sensitivity simulations (i.e. SPRING_PROF, SUMMER_PROF, and SUMMER_CIFS) with the results from the BASE simulation, the effects and persistence of model initialization could be studied for 67 days in spring and 72 days in summer. In all four simulations, initialization of the bidirectional model for NH_3 relied on NH_4^+ and H^+ concentrations simulated by the Environmental Policy Integrated Climate (EPIC) model (Williams et al., 1984, 2012) as described in Cooter et al. (2012), Pleim et al. (2013) and Bash et al. (2013). For the BASE, SPRING_PROF, and SUMMER_PROF simulations, atmospheric concentrations were initialized using the default CMAQ profile summarized for selected species in Table 1. It should be noted that when this default profile was first developed, the top of the model was lower than the 50 mb top used in this study and many other recent applications. For the SUMMER_CIFS simulation, atmospheric concentrations were initialized from the global C–IFS fields rather than the default CMAQ profile to investigate whether potentially more realistic initial conditions might lead to faster convergence between the base case and sensitivity simulations. A comparison of results from the BASE simulation against observations and other regional-scale model simulations was presented in Solazzo et al. (2017). The SPRING_PROF and SUMMER_PROF simulations included a chemically inert initial condition tracer (hereafter referred to as ICT) that undergoes advection and diffusion but is not affected by chemistry, deposition or scavenging. The ICT mixing ratio was arbitrarily set to 50 ppb at the beginning of the sensitivity simulations throughout the modeling domain and there were no ICT emissions and lateral boundary conditions throughout the simulations. The addition of the ICT in the SPRING_PROF and SUMMER_PROF simulations had no effect on any of the other species simulated by CMAQ.

3. Analysis and results

3.1. Atmospheric concentration initialization

Fig. 1a–b shows time-height cross sections of domain maximum ICT mixing ratios for the spring and summer cases. As noted above, the ICT mixing ratio was set to 50 ppb throughout the domain at the start of the SPRING_PROF and SUMMER_PROF simulations (February 23, 0 GMT and June 21, 0 GMT). Near the surface, ICT mixing ratios >30 ppb (i.e. 60% of the initial value) can be found after ten days while it takes 25–30 days for mixing ratios to fall to below 0.5 ppb (1% of their initial value). The ICT persistence aloft is similar to the surface results for the summer case but shorter for the spring case when domain maximum mixing ratios drop to less than 0.5 ppb after about 12 days.

The longer persistence of the domain maximum ICT in the upper layers for the summer case suggests the presence of a slow moving circulation pattern. This is confirmed in Fig. 2a–d for the spring case and 2e-h for the summer case. Fig. 2a–c (e-g) show maps of