Atmospheric Environment 98 (2014) 283–289

Contents lists available at ScienceDirect

Atmospheric Environment

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

Two reduced form air quality modeling techniques for rapidly calculating pollutant mitigation potential across many sources, locations and precursor emission types

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HIGHLIGHTS

- Two reduced form versions of an air quality model are compared and evaluated.
- Both methods are used to estimate impacts of emission reductions from power plants.
- Important differences between the two methods are discussed.

ARTICLE INFO

Article history:
Received 2 June 2014
Received in revised form
14 August 2014
Accepted 19 August 2014
Available online 23 August 2014

Keywords:
CMAQ-DDM
Response surface model
Emission controls
$PM_{2.5}$
Ozone

ABSTRACT

Due to the computational cost of running regional-scale numerical air quality models, reduced form models (RFM) have been proposed as computationally efficient simulation tools for characterizing the pollutant response to many different types of emission reductions. The U.S. Environmental Protection Agency has developed two types of reduced form models based upon simulations of the Community Multiscale Air Quality (CMAQ) modeling system. One is based on statistical response surface modeling (RSM) techniques using a multidimensional kriging approach to approximate the nonlinear chemical and physical processes. The second approach is based on using sensitivity coefficients estimated with the Decoupled Direct Method in 3 dimensions (CMAQ-DDM-3D) in a Taylor series approximation for the nonlinear response of the pollutant concentrations to changes in emissions from specific sectors and locations. Both types of reduced form models are used to estimate the changes in O_3 and $PM_{2.5}$ across space associated with emission reductions of NO_x and SO_2 from power plants and other sectors in the eastern United States. This study provides a direct comparison of the RSM- and DDM-3D-based tools in terms of: computational cost, model performance against brute force runs, and model response to changes in emission inputs. For O_3, the DDM-3D RFM had slightly better performance on average for low to moderate emission cuts compared to the kriging-based RSM, but over-predicted O_3 disbenefits from cuts to mobile source NO_x in very urban areas. The RSM approach required more up-front computational cost and produced some spurious O_3 increases in response to reductions in power plant emissions. However the RSM provided more accurate predictions for $PM_{2.5}$ and for predictions of very large emission cuts (*e.g.* −60 to −90%). This comparison indicates that there are some important differences in the output of the two approaches that should be taken under consideration when interpreting results for a given application.

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1. Introduction

Over the last few decades, air quality has improved substantially in most of the United States, Europe, and elsewhere. In the US, ambient air concentrations of regulated trace pollutants such as ozone (O_3), particulate matter (PM), carbon monoxide, nitrogen dioxide, sulfur dioxide (SO_2), and lead have all decreased (US-EPA,

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http://dx.doi.org/10.1016/j.atmosenv.2014.08.046
1352-2310/Published by Elsevier Ltd.

2012). This was possible from better scientific understanding of the physical and chemical processes governing the formation of these pollutants in the troposphere and the subsequent enactment of air pollution control policies of emission reductions and the emergence of cleaner technology. Still, millions of people in the US are routinely exposed to air pollutant concentrations above the levels that have been shown to be associated with increased risks for cardiovascular and respiratory disease (Lepeule et al., 2012; Atkinson, 2013). Furthermore, elevated ambient air pollutant concentrations are also found to be harmful to agricultural crops (Booker et al., 2009) and to have a dramatic impact on visibility (Liu et al., 2012). Thus, further improvements in ambient air quality would be clearly beneficial to both human health and welfare.

Sources for additional incremental reductions in air pollutant concentrations over what has already been achieved can be difficult to identify and prioritize. For this reason, numerical air quality models have been used as a testbed for quantifying the impacts of prescribed emission reductions to arrive at physically and economically feasible strategies for reducing ambient concentrations of O_3 and PM. One of these is the Community Multiscale Air Quality (CMAQ) model, which is widely employed by scientific institutes and regulatory agencies (www.cmaq-model.org). Traditionally, such models simulate the "base" level of pollution under current levels of emissions, and, then, repeat the simulation for emission levels proposed under a specific control strategy. The difference (or ratio for attainment demonstrations) between the "brute force" simulations at any receptor of interest is then assumed to be the impact of the control strategy. However, it is often extremely computationally intensive to apply state-of-the-science air quality models, such as CMAQ, to large geographic regions and long pollution episodes. Therefore, it is often resource prohibitive to test a large number of control strategies. For this reason, various source sensitivity and source apportionment techniques have been developed to reduce the size of the numerical problem (Cohan and Napelenok, 2011). Two of these techniques are developed and applied here to demonstrate their use for hypothetical emission reductions of a number of different types of sources over the eastern United States. The first is the response surface model approach (RSM; US-EPA, 2006), which aims to describe, using multidimensional kriging across the space defined by the range of potential emission reductions, the full pollutant concentration response to changes in emissions as a function of preselected control variables from a sufficiently large set of brute force simulations. The second is the Taylor series expansion of the concentration/emission function based on the model sensitivity coefficients calculated by the Decoupled Direct Method in three dimensions (DDM-3D). Both techniques are applied for a domain over the eastern United States, in order to quantify the impact on O_3 and $PM_{2.5}$ levels from hypothetical reductions to state specific emissions from electric generating units (EGUs) as well as domain-wide emission cuts to mobile, area, and other sources.

2. Method

All simulations for both methods were conducted using CMAQ version 4.7.1 (Foley et al., 2010) for August 2005 over the eastern United States at 12 km horizontal grid resolution and 14 vertical layers. The standard model configuration was used including the carbon bond version 2005 chemical mechanism (Sarwar et al., 2008). Boundary conditions were derived from another simulation over a larger encompassing 36 km domain. Boundary conditions for the 36 km simulation were obtained from a 2005 global GEOS-Chem simulation (http://wiki.seas.harvard.edu/geos-chem/). Emission inputs were developed using the Sparse Matrix Operator Kernel Emissions (SMOKE) processing system version 2.4 (http://www.smoke-model.org) based on the 2005 National Emissions Inventory and included year-specific data from the Continuous Emission Monitoring measurements from combustion and industrial processes. Emission summaries from the 2005 NEI for the sectors and pollutants of interest in this study are provided in Table S1 and Fig. S1 in the supplemental material. Meteorological inputs were processed using the Weather Research and Forecasting (WRF) model version 3.0 (Skamarock et al., 2008). Additional information regarding the modeling platform can be found in US-EPA (2013).

2.1. Development of a RSM-based reduced form model for CMAQ

Previous studies have demonstrated the use of response surface modeling techniques for the CMAQ model to estimate the human health benefits of reducing emissions from different sources in nine urban areas in the US (Fann et al., 2009), to compare the effectiveness of local and regional NO_x and VOC controls in three megacities in China (Xing et al., 2011), and to quantify the contribution of NH_3 emissions to fine particles in heavily developed regions of China (Wang et al., 2011). The response surface model developed here was used to estimate air quality impacts associated with emission reductions of NO_x and SO_2 from EGUs and other pollutants from other sectors in the eastern United States. The RSM was designed to provide state-specific information on the impacts of statewide shifts in emissions due to EGU policies, such as trading programs, and can also be used as a screening tool for comparing emission control strategies for attainment demonstrations.

The first step in developing an RSM is the selection of the source/emission factors that are of interest for a given application, i.e., experimental design. Here the RSM was developed to evaluate shifts in NO_x and SO_2 emissions at the state level for the EGU sector, while accounting for interactions with regional emissions of NO_x, SO_2, VOC, and NH_3 emissions from mobile, area (*e.g.*, agriculture, residential heating, dust), and non-EGU point sources (*e.g.*, industrial boilers, cement kilns). Although understanding state-specific EGU emission shifts was the focus of this study, it was not computationally feasible to designate separate emission factors for each of the states within the modeling domain. As a solution, the 42 states (including D.C.) are grouped into 15 clusters of one to three states, in order to reduce the total number of brute force simulations needed to create the RSM. States were grouped *a priori* based on zero-out simulations and SO_2 tracer model experiments such that the impact from emission cuts in any state would have minimal influence on the other states in its group. For example Group 1 consists of AR, PA and MT (the full group listings are provided in Fig. S2 in the supplemental material). In this way, although the emission factors for EGU emissions are based on state groups, it is still possible to estimate the air quality impacts of emission cuts in a single state. The final RSM experimental design consisted of 36 emission factors as shown in Table 1, mainly aimed at predicting the response of $PM_{2.5}$.

The RSM was designed to model changes in the predetermined emission factors ranging from 0% to 120% of base emission levels. This means the design space of interest was the 36 dimensional hypercube $[0, 1.2]^{36} \subset \mathbb{R}^{36}$. A two stage sampling design was used to

Table 1
Source/emission factors used in the design of the CMAQ RSM.

Sector	Geographical source	Pollutant	# emission factors
EGU	15 state cluster groups	NO_x, SO_2	30
Mobile	Domain wide	NO_x, VOC, NH_3	3
Area	Domain Wide	NH_3	1
Non-EGU	Domain Wide	NO_x, SO_2	2