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Multi-criteria selection of an Air Quality Model configuration based on quantitative and linguistic evaluations

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ABSTRACT

This study presents the application of multi-criteria evaluation in the selection of an optimal configuration for an Air Quality Model. The simulation domains focus on the Mexico City Metropolitan Area. A set of 10 different configurations were considered as alternatives. These configurations included convective parameterization, 6th order diffusion and exclusion of data assimilation within the Planetary Boundary Layer. In addition, model integration in a continuous setup and in a segmented setup was also considered. The modeling variables were surface temperature, wind speed, wind direction, and sulfur dioxide. The performance of the meteorological fields was evaluated with statistical metrics together with the Local Trend Association measure and further used as criteria. The air pollution field was evaluated qualitatively with five expert-based linguistic criteria and further converted into numerical terms. Meteorological variables and sulfur dioxide were aggregated into two single arrays, one for representing meteorology and the other for representing transport of a large industrial plume. Pareto Fronts were constructed for these two arrays under different weights scenarios. Results suggested that a model with no parameterizations in continuous integration setup and a model with segmented integrations using 6th order diffusion were the optimal configurations to conduct future air quality studies.

1. Introduction

It has long been recognized the negative impacts of air pollution on human health and ecosystems. The role of anthropogenic emissions is at the forefront of these impacts (WMO, 2012). To effectively address the air pollution at several spatial scales, air quality modeling is of utmost relevance. Air quality forecasting uses source and receptor models to study the degree of pollution in future events. There are several approaches to model air pollution, and all of them rely on the scientific goals under study which include the spatial scale of interest. In this respect, expert-based approaches are important in air quality studies. For example: in forecasting air pollution with fuzzy time series methods (Domanska & Wojtylak, 2012); classifying concentrations of criteria pollutants in Mexico (Barrón-Adame, Cortina-Januchs, Vega-Corona, & Andina, 2012); for controlling emissions (Zhou, Huang, & Chan, 2004), identification of geographical distribution of particle pollution (Li & Shue, 2004); or in suggesting a system for air quality management at regional scale based on interval programming with stochastic variables (Cao, Huang, & He, 2011).

Another approach consists in the application of deterministic models which solves the conservation equations of different physical and chemical processes (Zhang, Bocquet, Mallet, Seigneur, & Baklanov, 2012). These models are known as Air Quality Models (AQM) or Chemical Transport Models (CTM). This kind of models combines in a systematic approach current knowledge of meteorology, emissions and atmospheric chemistry to make forecasts of ambient concentrations (Molina et al., 2004). In addition, they provide scientific understanding of pollutant processes; can address and track, both in space and time, the long range transport of air pollutants; and can help in formulating scenarios involving changes in meteorology or emissions (Zhang et al., 2012). In Mexico, air quality studies using this type of models have been conducted in recent years focusing on different research objectives and on different kind of pollutants: sensitivity of ozone formation to emission changes (Lei, de Foy, Zavala, Volkamer, & Molina, 2007); assessment of possible underestimation of volatile organic compounds in the official National Emissions Inventory (West et al., 2004) and estimation of source contribution of large sulfur dioxide plumes (de Foy et al., 2009) among others.

Meteorological fields, including wind, hourly temperature, mixing depth and solar insolation fields are an important input for any modeling exercise with Air Quality Models (Russell & Dennis, 2000). These fields can have great uncertainty which contribute

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in mispredicting airborne chemical species, aerosols and particulate matter (Seaman, 2000). Thus, accurate meteorological fields in a CTM are of utmost importance. They will lead to reliable forecasts of air pollution events.

Multi-criteria evaluation is suitable for addressing complex problems involving high uncertainty, conflicting objectives and different data among other features (Wang, Jing, Zhang, & Zhao, 2009). It selects the best choice in a set of potential alternatives (Dalalah, Hayajneh, & Batieha, 2011). Since it is unlikely to achieve optimal values in all objectives at the same time, the final solution is a compromise of the initial alternatives in the selection process (Behnamian, Ghomi, & Zandieh, 2009). In environmental sciences it has been used in the development of a support system to help planning water resources management in the Haihe river (China) (Weng, Huang, & Li, 2010) and in the estimation of the optimum number of parameters for the coupled system of a multi-layer perceptron and the Numerical Weather Prediction (NWP) model HIRLAM (Niska et al., 2005). In this respect, the best configuration for either a NWP or a CTM cannot be known a priori, even though there are recommended parameterizations which produce reliable results. Therefore, sensitivity experiments are conducted in order to choose the best configuration among different physical parameterizations (Borge, Alexandrov, del Vas, Lumbreras, & Rodríguez, 2008; Lo, Yang, & Pielke, 2008). However, not all the possible combinations are feasible to be evaluated since some parameters are specific for some modeling options. Although sensitivity studies usually focus on the meteorological fields, there are works which additionally assess the potential transport of pollutants for each configuration. Trajectory calculations are computed in order to evaluate the meteorological fields (Godowitch, Gilliam, & Rao, 2011; Ngan et al., 2012; Seaman, 2000). This allows depicting the degree of uncertainty in the meteorological fields. Nevertheless, the plume transport is not considered in these works as an extra criterion to evaluate model performance.

The main objective of this study is to select an optimum configuration for an AQM based on multi-criteria evaluation. The main motivation is to have a trade-off between meteorology and plume transport in order to conduct a regional air quality simulation focusing on the Mexico City Metropolitan Area (MCMA). Section 2 presents the AQM and the area of study. The methodology is presented in Section 3. Results and discussion are given in Section 4, and conclusions of this study are summarized in Section 5.

2. Air Quality Model and area of study

2.1. WRF-Chem

Detailed Eulerian numerical Air Quality Models have been developed for research purposes and to support emissions-control policy decisions (Seaman, 2000). An example is the WRF-Chem model. It is an on-line chemistry model fully coupled to the Weather Research and Forecasting (WRF) model (Skamarock et al., 2005) with lead developments at the National Oceanic and Atmospheric Administration (NOAA) and the Pacific Northwest National Laboratory (Fast et al., 2006; Grell et al., 2005). In this respect, the WRF model is a state-of-the-art mesoscale system designed for both short- and long-term weather and climate simulations. It is a non-hydrostatic model, with different physical parameterizations, including cumulus parameterizations, Planetary Boundary Layer, land surface models, long-wave and short-wave radiation, and microphysics models. It also includes multi-scale data assimilation. Thus, the WRF-Chem preserves the transport, grid and physics schemes of WRF's meteorological component when solving the transport in sub-grid scales. It has different chemical mechanisms, as well as several schemes of aerosol and photolysis (WRF-Chem, 2010; WRF, 2010). WRF-Chem version 3.2.1 is used in the present study.

2.2. Tula region and MCMA

The city of Tula is located in the Mezquital Valley, in southwest Hidalgo with a total population of nearly 94,000 inhabitants and more than 140 industries. The region is semi-arid with average temperatures of 17 °C and precipitation ranging from 432 to 647 mm, increasing from north to south. In this region, the Tula Industrial Complex is settled in an area of 400 km^2. The major industries of the city are located within this region, including the Miguel Hidalgo Refinery, the Francisco Perez Rios power plant, several cement plants and limestone quarries. Other minor industries include metal manufacturing, processed food, chemical and incineration of industrial waste. The emission of pollutants from combustion processes of these industries impacts the regional air quality. In addition, the inflow of untreated sewage water from Mexico City promotes severe pollution problems to soil and water resources (Cifuentes, Blumenthal, Ruíz-Palacios, Bennett, & Peasey, 1994; Vazquez-Alarcon, Justin-Cajuste, Siebe-Grabach, Alcantar-Gonzalez, & de la Isla-de Bauer, 2001). According to current environmental regulations, this region is classified as a critical area due to the high emissions of SO_2 and particulate matter (SEMARNAT-INE, 2006).

The MCMA is the largest megacity in North America, and the third largest urban agglomeration, with nearly 22 million inhabitants, after Tokyo (Japan) and Delhi (India) (UN, 2012). It is located in the subtropics within an elevated U-shaped basin surrounded by mountain ridges which border the west, east and south regions of the city. The metropolitan area covers 1500 km^2 on the southwest side (Parrish, Singh, Molina, & Madronich, 2011; Williams, Brown, Cruz, Sosa, & Streit, 1995). This topography acts like a barrier to large-scale circulations and isolates the basin from the winds of synoptic weather systems at low levels (Zhang & Dubey, 2009). Previous work has shown that emissions from Tula Industrial Complex can impinge into the megacity, exerting an influence on sulfur dioxide pollution levels in the city (de Foy et al., 2009; Williams et al., 1995; Almanza, Molina, & Sosa, 2012).

3. Air Quality Model configurations

A set of 10 different WRF-Chem configurations were considered in this study. Each model run encompass a 6-day simulation period, from 00:00 UTC 22 March to 00:00 UTC 28 March of 2006, using three domains with horizontal resolution of 27, 9 and 3 km, and 35 vertical levels (Fig. 1a). All of the simulations performed Multiscale Four Dimensional Data Assimilation (FDDA) to improve accuracy in the meteorological fields and keep the same physics to maintain consistency. Operational meteorological data, Mexico City Air Quality Network (RAMA) surface data; and radar wind profilers, radiosondes and surface data from MILAGRO field campaign were used in the FDDA assimilation process. MILAGRO field campaign was a major international collaborative project to examine the behavior and export of atmospheric emissions from the Mexico megacity (Molina et al., 2010).

The simulations considered two of the main approaches to run an AQM. The first one of them is a single continuous integration requiring an initialization of meteorology and chemistry just at the beginning of the run. The second one is a multiple integration of overlapping short segments requiring multiple initializations at the beginning of each segment run. Even though they appear similar, final results may differ. In addition, computing time and disk storage are important features to take into account when running the AQM in either of these approaches. Segmented runs tend to require relatively more disk space than a single continuous run.