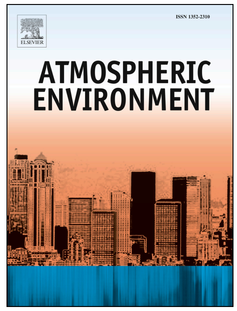
Accepted Manuscript



Impact of time-dependent chemical boundary conditions on tropospheric ozone simulation with WRF-Chem: An experiment over the Metropolitan Area of São Paulo

M. Gavidia-Calderón, A. Vara-Vela, N.M. Crespo, M.F. Andrade

PII: S1352-2310(18)30621-6

DOI: 10.1016/j.atmosenv.2018.09.026

Reference: AEA 16259

To appear in: *Atmospheric Environment*

Received Date: 29 March 2018

Revised Date: 14 September 2018

Accepted Date: 16 September 2018

Impact of time-dependent chemical boundary conditions on tropospheric ozone simulation with WRF-Chem: An experiment over the Metropolitan Area of São Paulo.

M. Gavidia-Calderón [a]*, A. Vara-Vela [a], N. M. Crespo [a], M. F. Andrade [a]
[a] Department of Atmospheric Sciences, Institute of Astronomy, Geophysics and Atmospheric Sciences, University of São Paulo, São Paulo, Brazil

Abstract

WRF-Chem (Weather Research and Forecasting with Chemistry Model) is being used to perform air quality forecast over the southeast Brazil with a domain centered in the Metropolitan Area of São Paulo (MASP). The simulations are used to understand the pollutants behavior concerning the fluxes to and from the urban areas, to examine the formation of secondary pollutants (e.g., tropospheric ozone), and to validate the efficacy of air quality policies implementation, particularly the ones that are related to the vehicular fuel used in the region. One important factor to improve the air quality simulations is the configuration of suited inflow boundary conditions for the chemical species. In that context, the objective of this study is to assess the impacts of using time-dependent Chemical Lateral Boundary Conditions (CBC) on tropospheric ozone simulations with WRF-Chem. Two simulations were carried out using Carbon-Bond Mechanism version Z (CBMZ). The first simulation was a set-up to run with WRF-Chem default CBC, and the second one using time-dependent CBC obtained from MOZART-4 (Model for Ozone and Related chemical Tracers, version 4) simulations. The period of study was from May 15 to May 18 and from October 30 to November 1, 2006, when a comprehensive experiment with ozonesondes launching and surface measurements was performed. Results show that using MOZART-4 CBC reduced mean bias, RMSE and slightly improved correlation coefficients for ground level ozone as well as ozone vertical profile above 3 km. These improvements were more significant during periods with lower photochemical activity. However, underestimation of ozone concentration peaks was also observed in this period, which can be an issue for operational air quality forecasting.

Keywords: Chemical boundary conditions, WRF-Chem, MOZART-4, Tropospheric Ozone, São Paulo megacity.

1. Introduction

Air pollution is among the first ten risk factors for disease burden (Lim et al., 2013) and is also one of the biggest problems that affects megacities all over the world, where high ozone and particulate matter concentrations are frequently experienced (Baklanov et al., 2016). In South America, the most populated megacity is the Metropolitan Area of Sao Paulo (MASP) with a population above the 20 million inhabitants (United Nations, 2014). According to São Paulo State Environmental Agency (CETESB), tropospheric Ozone (O_3) and Fine Particulate Matter ($PM_{2.5}$) are the pollutants that frequently exceed the state air quality standards (i.e., 140 µg/m^3 or ~70 ppb of 8 hour moving average and 60 µg/m^3 of daily mean, respectively). In 2017, the ozone concentrations were above the state air quality standard for 28 days and exceeded the national air quality standard (160 µg/m^3 or ~80 ppb of hourly concentration) for 68 days (CETESB, 2018).

Long-term analysis of pollutants concentration in MASP showed a decrease in the primary pollutants, such as CO, NO_x and SO_2. However, an increase in the number of days with Ozone standard exceedance has been indicated (Carvalho et al., 2015; Perez-Martinez et al., 2015 and Andrade et al., 2017). MASP is highly influenced by vehicular emissions of more than 7 million cars (CETESB, 2018): 3% of which are heavy-duty vehicles fueled with bio-diesel, 85% light duty vehicles running on gasohol (gasoline with 25% of ethanol) or hydrated ethanol (95% ethanol and 5% water), and 12% motorcycles. Some studies attempted to evaluate the impact of using ethanol or gasohol on the Maximum Incremental Reactivity for ozone formation. Alvim et al. (2017), identified using the Ozone Isopleth Package for Research (OZIPR), that the main ozone precursors are formaldehyde, acetaldehyde and