Environmental Modelling & Software 59 (2014) 127–134

Contents lists available at ScienceDirect

Environmental Modelling & Software

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

Simple atmospheric dispersion model to estimate hourly ground-level nitrogen dioxide and ozone concentrations at urban scale

Andrea L. Pineda Rojas*

Centro de Investigaciones del Mar y la Atmósfera (CIMA/CONICET-UBA), DCAO/FCEN, UMI-IFAECI/CNRS, Ciudad Universitaria, Pab.II piso 2, 1428 Buenos Aires, Argentina

ARTICLE INFO

Article history:
Received 1 March 2014
Received in revised form 17 May 2014
Accepted 21 May 2014
Available online

Keywords:
Buenos Aires
DAUMOD-GRS model
Nitrogen dioxide
Ozone
Urban air quality modelling

ABSTRACT

Atmospheric nitrogen dioxide (NO_2) and ozone (O_3) present potential health risk at large urban centres worldwide. Modelling their ground-level concentrations is a fundamental part of urban air quality assessment studies. Simple atmospheric dispersion models are particularly useful in places lacking detailed input data to run complex models and for applications requiring a large number of simulations, also allowing high spatial and temporal resolution even for long-term calculations. The DAUMOD-GRS urban atmospheric dispersion model has been developed aiming to have these features. This work presents its performance evaluation considering hourly concentrations of NO_2 and O_3 measured at twenty sites across the Metropolitan Area of Buenos Aires (MABA), Argentina. Results show an acceptable model performance, with a small tendency to underestimate NO_2 and to overestimate O_3. By grouping the monitoring sites in regions having different emission conditions, it is found that the model reproduces well the observed urban-suburban concentration gradients.

1. Introduction

Urban concentrations of nitrogen dioxide (NO_2) and ozone (O_3), resulting from anthropogenic emissions of nitrogen oxides (NO_x) and volatile organic compounds (VOC), may cause adverse effects on human health if they are relatively high (WHO, 2005). Therefore, evaluation of their ground-level concentrations is fundamental in urban air pollution assessment studies, for which modelling plays an essential role. Deterministic urban air quality models (UAQMs) are commonly used to estimate urban background concentrations. They are based on mathematical relationships that describe the processes involved in the formation, transport and dispersion of air pollutants. Since these models provide a link between the emissions of primary species and the concentrations of secondary (formed) compounds, they are useful to identify the various source contributions, and to evaluate the impact of different emission abatement strategies on pollutant levels. In addition, UAQMs provide the input for street canyon models which allow the assessment of human population exposure, and hence they are also an important component of integrated assessment models (e.g., Finardi et al., 2008; Leksmono et al., 2006; Mensink and Cosemans, 2008; Namdeo et al., 2002; Sokhi et al., 2008).

Usually, UAQMs can be classified into comprehensive and simple semi-empirical models (Moussiopoulos, 2003). A detailed representation of simulated processes behind the production/loss of a pollutant may help to understand the interactions among emissions, atmospheric conditions and pollutant chemistry in the urban atmosphere. In this sense, the capabilities and performance of advanced numerical UAQMs have been improved substantially in the last years (Borge et al., 2008). However, increasing the complexity of models can introduce more parameters with uncertain values, decreasing transparency and increasing overall uncertainty (Derwent et al., 2010). The lack of detailed input data is one of the main sources of uncertainty of the deterministic models. For example, the chemical species of the emission inventories must match those of the chemical mechanism included in the UAQM. Thus, a greater number of reactions and species requires a greater knowledge of the pollutants (both their emissions and regional background concentrations) involved in the mechanism, which may not be available. On the other hand, the degree of complexity also influences the number of simulations that can be performed, which is particularly important for regulatory purposes involving hundreds of model runs. In cases like these, simple models provide an acceptable alternative to estimate urban background concentrations. In places where there is not enough available information to run comprehensive models, they may constitute the only tool to gain some insight into the source-receptor relationships. In urban

* Tel.: +54 11 4787 2693.
E-mail address: pineda@cima.fcen.uba.ar.

http://dx.doi.org/10.1016/j.envsoft.2014.05.016
1364-8152/

areas where the input data are not a limitation, simple UAQMs can be used to obtain a large number of simulations that allow a selection of a few scenarios to be then run with comprehensive models.

The DAUMOD model (Dispersión Atmosférica Urbana, in Spanish) (Mazzeo and Venegas, 1991) is a simple urban atmospheric dispersion model for area sources that was originally designed for inert species. Different versions of DAUMOD were developed during the last two decades to study several aspects of the urban air quality in the Metropolitan Area of Buenos Aires (MABA), Argentina (e.g., Mazzeo and Venegas, 2008; Mazzeo et al., 2010; Pineda Rojas and Venegas, 2009; Venegas and Mazzeo, 2006; Venegas et al., 2011). The MABA, which is composed by the City of Buenos Aires (CBA, ~200 km^2) and the Greater Buenos Aires (GBA, ~3600 km^2), is the third megacity of Latin America and the twelfth worldwide (United Nations, 2012). It is located on a flat terrain, mainly surrounded by non-urban areas. A few campaigns carried out in the CBA and air quality modelling studies have shown that urban background concentrations of NO_2 and O_3 are lower than their corresponding air quality standards, but NO_2 hourly levels may exceed the World Health Organisation air quality guideline at some places in the MABA (see Venegas et al., 2011). The DAUMOD-GRS model arises from the need to improve the NO_2 DAUMOD estimations. Based on its structure and taking into account the lack of detailed information available for the MABA (especially in relation to emission data), the DAUMOD model was coupled with a simplified photochemical scheme, the Generic Reaction Set (GRS) (Azzi et al., 1992). The GRS has been included already in some atmospheric dispersion models [e.g., ADMS-Urban (CERC, 2001), TAPM (Hurley et al., 2005), CIT (Lashmar and Cope, 1995), SOMS (Venkatram et al., 1994)] due to its simplicity and ability to reproduce the interactions between NO_2 and O_3 at urban scale. In a previous paper (Pineda Rojas and Venegas, 2013a), the development of the DAUMOD-GRS model and its first application in the CBA was presented. Recently available NO_2 and O_3 concentration data from twenty sites distributed outside the city have allowed a more complete evaluation of its performance in the area. In Pineda Rojas and Venegas (2013b), a study of the model ability to simulate O_3 in the MABA, focussing on the summer maximum diurnal peak concentrations, has been presented. The present work discusses the performance of DAUMOD-GRS to estimate hourly urban background NO_2 and O_3 concentrations considering observations from twenty sites in the MABA. The statistical comparison is carried out by grouping the monitoring stations in regions having different emission conditions, in a way that allows the evaluation of the modelled and observed urban-suburban concentration gradients, and the examination of the validity of the assumption of spatial homogeneity of atmospheric variables for this modelling application.

A brief description of the DAUMOD-GRS structure is presented in Section 2. Section 3 comments on the evaluation procedure and the choice of evaluation metrics and method. Section 4 summarises the data used to perform the statistical evaluation of the model, the running conditions and the results obtained. Finally, a discussion on model assumptions and their likely impact is presented in Section 5, followed by the conclusions in Section 6.

2. The DAUMOD-GRS model

The DAUMOD-GRS model was developed by coupling of the DAUMOD model with the GRS scheme. It is written in FORTRAN and due to its simple configuration and low computational demand, it can be run on any personal computer. The description of the two main components (DAUMOD and GRS) and their coupling can be found in Pineda Rojas and Venegas (2013a). Here, its main assumptions and structure are summarised (see Fig. 1).

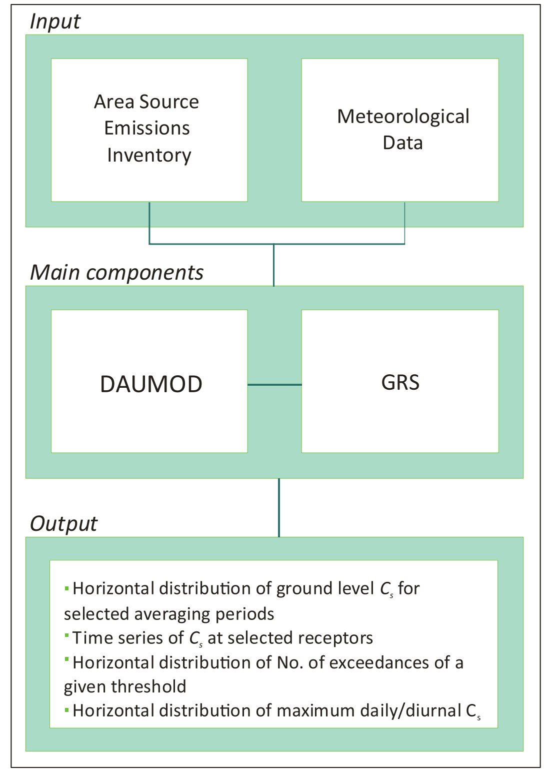

Fig. 1. Structure of the DAUMOD-GRS model (C_s: concentration of species s: NO, NO_2, O_3).

2.1. Input module

The model takes into account information regarding the domain characteristics: grid size, latitude and longitude of the domain centre, meteorological conditions, the distributions of area source emissions of NO_x and VOC and their speciation, background concentrations of the species involved in the GRS, surface roughness. These data and the running conditions (spatial and temporal resolutions and period of the simulations) are read from an input file.

2.2. Transport and dispersion module

Given a horizontal distribution of NO_x and VOC emissions from multiple area sources, their atmospheric transport and dispersion is first computed by the atmospheric dispersion model DAUMOD (Mazzeo and Venegas, 1991). The DAUMOD model is based on the equation of mass continuity and assumes the x-axis in the mean wind direction, the z-axis vertical and no transport of mass through the upper boundary of the pollutant plume. The expression used by the model to estimate the concentration of a species s, at a downwind distance x and ground-level ($z = 0$), due to atmospheric dispersion and transport from an area source i of uniform emission strength $Q_{s,i}$ located between $x = x_{i-1}$ and $x = x_i$, is:

$$C_{s,i}(x,0) = aQ_{s,i}\left[(x-x_{i-1})^b - (x-x_i)^b\right] \Big/ \left(|A_1|kz_0^b u_*\right) \quad (1)$$

where k is the von Karman constant (=0.41), u_* is the friction velocity, z_0 is the surface roughness length and a, b and A_1 are coefficients that depend on the atmospheric stability (expressions in Venegas and Mazzeo, 2006). It follows that the pollutant ground-level concentration due to a horizontal distribution of N area sources located upwind the receptor, is given by: