Atmospheric Environment 80 (2013) 152–160

Contents lists available at ScienceDirect

Atmospheric Environment

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

Dispersion of an urban photochemical plume in Phoenix metropolitan area

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HIGHLIGHTS

- Dispersion and chemistry of an urban plume were explained using MM5–CMAQ models.
- An urban plume can be described in terms of "inert" and "active" dispersion.
- The inert dispersion, exemplified by CO, takes the form of a Gaussian-like plume.
- Still, it is subjected to heterogeneities of topography and flow patterns.
- The active dispersion leads to a different shape, depending on chemical reactivity.

ARTICLE INFO

Article history:
Received 3 November 2012
Received in revised form
25 July 2013
Accepted 28 July 2013

Keywords:
Dispersion of an urban plume
Inert passive dispersion
Active dispersion
Ozone
Photo-oxidants
CMAQ
MM5

ABSTRACT

Air quality simulations were conducted using MM5/CMAQ modeling platform to study the intricacies introduced by photochemical reactions during the dispersion of urban pollution plume of Phoenix metropolis. The simulation days included the sole ozone episode recorded during 1996–2005, which violated the previous 1-h ozone standard (0.12 ppm). The modeling results suggest that the Phoenix urban plume can be described in terms of "inert passive dispersion" and "chemically active dispersion". The former is exemplified by the CO distribution and takes the form of a Gaussian-like plume, for which the source is located at the ground level of the urban core or a freeway. The passive dispersion, nevertheless, is directly subjected to heterogeneities of topography and flow patterns, and hence cannot be strictly Gaussian. The case of active dispersion is much more complicated, and leads to a different plume shape, depending on the chemical reactivity of pollutant species. Secondary pollutants such as ozone and its precursors cause the plume core to have its maximum concentration far downwind of the urban area. Chemical species such as VOCs, which are directly emitted from a source as well as transformed by other primary pollutants, form a plume that qualitatively resembles a transition from an inert plume (CO) to a highly reactive plume (NO_x).

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1. Introduction

Ozone is one of the six regulated (criteria) pollutants by the US Environmental Protection Agency (EPA), and complying with EPA's ozone standard is considered the most challenging of all environmental regulations for certain geographical areas. Numerous major urban centers in the United States have long histories of non-attainment of National Ambient Air Quality Standards (NAAQS) for ozone, and the prospect of complying in the near future is bleak, some reasons being that the regulatory standards are becoming more stringent, and anthropogenic activities are increasing. Once thought to be confined to urban centers, ozone is now recognized to be prevalent in suburbs and rural areas, with comparable or higher concentrations in areas downstream of urban centers than in the urban centers themselves (Lu and Turco, 1996; Fast et al., 2000; Lee et al., 2003, 2007). The transport of ozone and related oxidants from urban to rural areas, thus appears to be crucial for air quality studies. In addition, pollutants can be lifted up by convection and incorporated into regional and global scale flows (Fernando et al., 2010), which is of current concern because of perceived wide-ranging impacts on human and ecosystem health, agriculture, visibility degradation, weather modification, radiative forcing and tropospheric oxidation capacity (Fernando, 2010).

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1352-2310/$ – see front matter Published by Elsevier Ltd.
http://dx.doi.org/10.1016/j.atmosenv.2013.07.066

There are many studies that deal with ozone and photo-oxidants in urban areas (Zaveri et al., 2003; Gaffney et al., 2002; Kleinman et al., 2003) or within a rural air mass (Olszyna et al., 1994), either focusing on photochemistry or transport and mixing of urban pollutants (Banta et al., 1997; McKendry et al., 1997; Fast et al., 2000; Solomon et al., 2000; Doran et al., 2003; Lee et al., 2003, 2007). Only a few previous studies, however, have presented an integrated picture describing the transport of an urban plume that undergoes complex chemical reactions, while being subjected to advection and diffusion within the surface and entire atmospheric boundary layer (Shi et al., 2009).

This paper concerns the physical and chemical processes that govern the transport of air pollutants from an urban center to rural neighborhoods, focusing on the structure and characteristics of the plume by analyzing the transport of and chemistry within the plume. To this end, we have employed the Penn State/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) and the U.S. EPA's chemical transport model (Community Multi-scale Air Quality Model, CMAQ). Numerical simulations and subsequent analysis were conducted for the Phoenix metropolitan area, which is currently designated as an 8-hr ozone non-attainment area.

2. Numerical models and their configurations for simulations

MM5 version 3 (Grell et al., 1995) was employed to simulate meteorological fields for chemical transport modeling. These simulations were performed with 4 nested domains, with respective grid resolutions of 54 km, 18 km, 6 km and 2 km. The innermost domain spans 164 km × 106 km in the E-W and N-S direction respectively, encompassing the Phoenix valley and surrounding mountains. Vertically, 26 layers were used, with the middle of the lowest computational layer being approximately 10 m above the ground level (agl). The Medium Range Forecast (MRF) Planetary Boundary Layer (PBL) scheme, cloud radiation, and simple ice microphysics scheme were chosen for the simulations, after carefully considering available options of MM5. Betts-Miller and Kain-Fritsch cumulus schemes were employed for domains 1 and 2, respectively, but no cumulus parameterization was used for the two inner domains, considering the dry weather conditions encountered. For the land surface scheme, the five-layer soil model was used, in which the temperature is predicted using a vertical diffusion equation for 0.01, 0.02, 0.04, 0.08, and 0.16 m deep layers from the surface, with the assumption of fixed substrate. The NCEP (National Center for Environmental Prediction) *Eta* model output (Grid 212 with 40 km spacing) was used to provide initial and boundary values for MM5 simulations, and the data assimilation was performed using NWS (National Weather Service) soundings and surface measurements. A period of 48 h of simulation was analyzed, following 48 h of spin-up.

The Eulerian photochemical model CMAQ version 4.1 was employed to simulate the concentrations of ozone and other oxidants. Two nested CMAQ domains, identical to the innermost two domains of MM5, were used except that several lateral boundary columns and rows were excluded in order to reduce uncertainty seeping from the lateral boundaries of the MM5 domain. Ozone, nitrogen oxides and carbon monoxide measurements from the Arizona Department of Environmental Quality (ADEQ) routine surface monitoring stations were interpolated to build 2-D concentration fields that were used as the initial and lateral boundary values for the outer domain; they were further refined using ozone and nitrogen oxides measured by a research aircraft during the Phoenix '98 field experiment (Fast et al., 2000). The aircraft samples were taken at the altitudes between 400 and 3000 m agl. Terrain heights in the modeling domain and the locations of ADEQ's air quality monitoring stations are presented in Fig. 1. The outer domain selected was sufficiently large to circumscribe a typical travel distance of an air mass driven by local thermal circulation, thus minimizing uncertainties associated with lateral boundary values. The results for the outer domain were used as the initial and boundary values for the inner domain. A model-ready emission inventory was provided by the ADEQ in Urban Airshed Model (UAM) format. The emissions inventory was originally developed for a regulatory application, Metropolitan Phoenix Voluntary Early Ozone Plan (ENSR, 1997). Wherein, the U.S. EPA's MOBILE model was used to estimate on-road vehicle emissions. Biogenic VOC and NO_x emissions were estimated using Maricopa Association of Governments' Biogenic Emissions Inventory System, Version 2 (MAGBEIS2, STI, 1996), which constitutes an improvement over the EPA BEIS2 procedures. This UAM-ready inventory was mapped to the CMAQ-ready species, and converted to I/O API format using an algorithm developed for the current study.

3. Episode days

The Phoenix metropolitan area is currently designated as an 8-h ozone nonattainment area under the U.S. EPA Clean Air Act. The

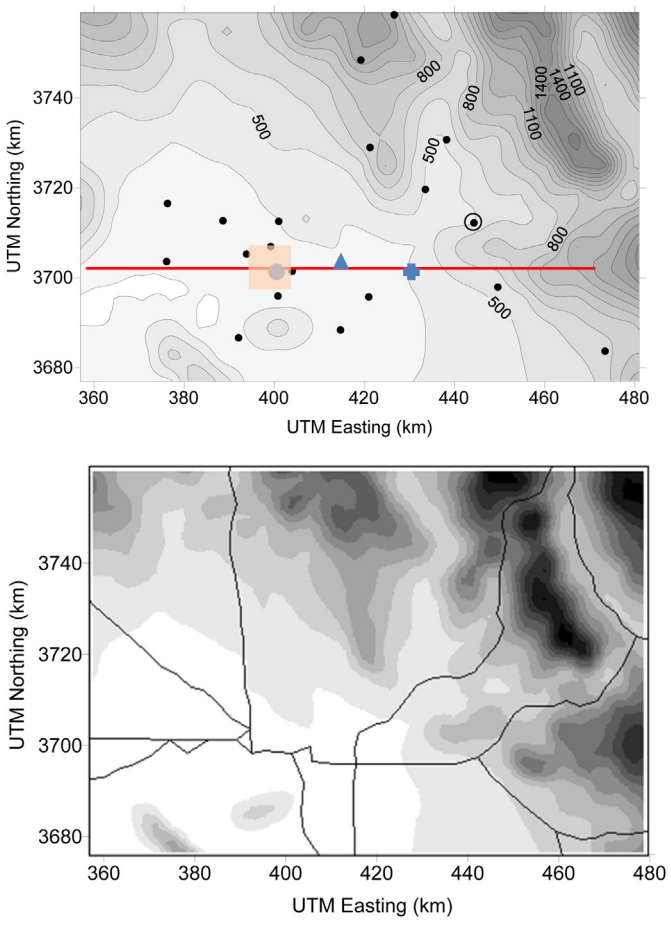

Fig. 1. The locations of the ADEQ air quality monitoring stations. Central Phoenix, South Scottsdale and Falcon Field are marked with a larger circle, triangle and thick plus symbol, respectively, while general downtown area is represented by a lightly shaded rectangle. The double circle represents the location of the highest O3 during the episode days. The gray shadings represent terrain elevation. The solid red line indicates the cross-section, along which the pollutant distributions are discussed in Section 5. Major roadways within the modeling domain are presented in the topographic map shown below (solid lines). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)