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Spatial variability of summertime tropospheric ozone over the continental United States: Implications of an evaluation of the CMAQ model

Daniel Q. Tong[a,*], Denise L. Mauzerall[a,b,**]

[a]Science, Technology and Environmental Policy Program, Woodrow Wilson School of Public and International Affairs, Princeton University, Princeton, NJ 08544, USA

[b]Geosciences Department, Princeton University, USA

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Abstract

This study evaluates the ability of the Community Multiscale Air Quality (CMAQ) model to simulate the spatial variability of summertime ozone (O_3) at the surface and in the free troposphere over the continental United States. Simulated surface O_3 concentrations are compared with 987 Air Quality System (AQS) sites and 123 Clean Air Status and Trends Network (CASTNet) sites. CMAQ's ability to reproduce surface observations varies with O_3 concentration. The model best simulates observed O_3 for intermediate concentrations (40–60 ppbv), while over-(under-) predicting at lower (higher) levels. CMAQ reproduces surface O_3 for a wide range of conditions (30–80 ppbv) with a normalized mean error (NME) less than 35% and normalized mean bias (NMB) lying between $\pm 15\%$ for the whole domain. Although systematically over-predicting O_3 in the east and under-predicting it in the western United States, CMAQ is able to reproduce 1- and 8-h daily maxima with a cross-domain mean bias (MB) of 1 and 8 ppbv, or NMB of 8% and 25%, respectively. The model underestimates observed O_3 at rural sites (MB $= -5$ ppbv, NMB $= -5\%$ and NME $= 23\%$ with a 40 ppbv cut-off value) and over-predicts it at urban and suburban sites by a similar magnitude (MB $= 6$ ppbv, NMB $= 7\%$ and NME $= 25\%$). Apparent errors and biases decrease when data is averaged over longer periods, suggesting that most evaluation statistics are dependent on the time scale of data aggregation. Therefore, performance criteria should specify an averaging period (e.g., 1- or 8-h) and not be independent of averaging period as some current model evaluation studies imply. Comparisons of vertical profiles of simulated O_3 with ozonesonde data show both overestimation and underestimation by 10–20 ppbv in the lower troposphere and a consistent under-prediction in the upper troposphere. Vertical O_3 distributions are better simulated when lateral boundary conditions obtained from the global Model of Ozone and Related Tracers version 2 (MOZART-2) are used, but under-prediction remains. The assumption of zero-flux at the top boundary and the resulting exclusion of the contribution of stratosphere–troposphere exchange to tropospheric O_3 concentrations limit the ability of CMAQ to reproduce O_3 concentrations in the upper troposphere.

Keywords: CMAQ; Model evaluation; Ozone; Ozonesonde; Vertical profile; Air quality model

*Corresponding author. Tel.: +1 919 541 5150.

**Also corresponding author. Tel.: +1 609 258 2439.

E-mail addresses: tong.daniel@epa.gov (D.Q. Tong), mauzeral@princeton.edu (D.L. Mauzerall).

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1. Introduction

Tropospheric ozone (O_3) continues to be a major concern for both the research and regulatory communities due to its importance in atmospheric chemistry (Logan et al., 1981) and climate change (Ramaswamy, 2001), as well as its harmful effects on public health (EPA, 1999; Bell et al., 2005; Ito et al., 2005; Levy et al., 2005), agriculture and ecosystems (Mauzerall and Wang, 2001; NRC, 2004). In an effort to protect public health and welfare, in 1971, the US Environmental Protection Agency (EPA) set the National Ambient Air Quality Standards (NAAQS) for O_3 at 0.12 ppmv for a 1-h daily maximum value. In 1997, EPA revised the O_3 NAAQS to require that a 3-year average of the annual fourth highest daily 8-h average concentration not exceed 0.08 ppmv. Despite these regulatory measures, there has been little progress in reducing nationwide O_3 levels in recent years (EPA, 2000; Lin et al., 2001). Between 1989 and 1998, there was only a 4% decrease in the national second highest daily maximum 1-h O_3 value and "no change" in the fourth highest daily maximum 8-h average (EPA, 2000). With the exception of the southwest, exceedances of both 1- and 8-h NAAQS have not significantly changed in the past decade, suggesting that air quality gains from the 1980s to 1990s have not continued (Lin et al., 2001). Compliance with the O_3 NAAQS within any state is complicated by inter-state transport. Long-range transport of O_3 and its precursors from upwind areas may contribute significantly to persistent nonattainment of the O_3 standards at many locations. The need to address inter-state transport of O_3 and its precursors has led to the formation of multi-state organizations to mitigate air pollution, including the Ozone Transport Commission (OTC) and the Ozone Transport Assessment Group (OTAG) (NRC, 2004), and most recently the Clean Air Interstate Rule (CAIR) in 2005 which is designed to reduce NO_x and SO_2 emissions in the eastern United States by capping regional emissions.

Air quality models are valuable tools for simulating the spatial distribution of O_3 concentrations, resulting from both local emissions and long-range transport of O_3 precursors, in locations where measurements are not available. In addition, they allow an exploration of emission control strategies to mitigate elevated concentrations of O_3, which can help states attain the NAAQS. The EPA's Models-3 Community Multi-scale Air Quality (CMAQ) model (Byun and Ching, 1999) has increasingly been used by both the regulatory and scientific communities to investigate these issues. However, evaluation of CMAQ's ability to reproduce the spatial distribution of surface O_3 is needed to assist interpretation of simulation results.

This paper evaluates the ability of CMAQ to reproduce O_3 measurements at the surface and in the troposphere over the continental United States. Most previous evaluations of CMAQ performance have focused on a single geographic area, including the eastern US (Hogrefe et al., 2001, 2004), the mid-Atlantic states (Bell et al., 2003), and the southeastern US (Kang et al., 2003). While informative, these studies have not analyzed the spatial variability of O_3 across the entire country. This paper, together with other emerging papers (e.g., Eder and Yu, 2005), evaluates model performance over the entire continental US in a consistent fashion. Our study focuses on CMAQ's ability to: (1) capture the spatial variability in surface O_3 concentrations, (2) accurately simulate O_3 concentrations in both rural and urban locations, and (3) reproduce high O_3 concentrations during pollution episodes as well as low concentrations in clean air. Furthermore, we (4) examine the influence that averaging time periods have on apparent model performance. Finally, we (5) evaluate the vertical distribution of tropospheric O_3 simulated by CMAQ and assess the impacts of lateral boundary conditions (LBC) on simulated O_3 concentrations at the surface and in the free troposphere using both a predefined LBC and an LBC obtained from the global Model of Ozone and Related Tracers version 2 (MOZART-2).

We describe the CMAQ model, measurements and methods used for model evaluation in Section 2. Evaluation results are presented in Section 3 and their implications for CMAQ applications are discussed in Section 4. We conclude in Section 5.

2. Model, observations and methods

2.1. CMAQ simulation

We use the CMAQ model (Dennis et al., 1996; Byun and Ching, 1999) version 4.2 to simulate the transport and chemical transformation of tropospheric O_3 and its precursors for July 1996 over the continental United States. CMAQ is a comprehensive Eulerian grid model that simulates the complex interactions among multiple atmospheric pollutants