EVALUATION OF CMAQ MODELING RESULTS USING SATELLITE REMOTE SENSING MEASUREMENTS OVER NORTH AMERICA

Krish Vijayaraghavan[1a], Jianlin Hu[2], Yang Zhang[2],
Xiong Liu[3], Kelly Chance[3], and Hilary E. Snell[1b]

[1]Atmospheric & Environmental Research, Inc. (AER), [a]San Ramon, CA, and [b]Lexington, MA
[2] North Carolina State University, Raleigh, NC
[3] Harvard-Smithsonian Center for Astrophysics, Cambridge, MA

1. INTRODUCTION

The evaluation of regional air quality models is typically conducted using ground-level measurements and limited data aloft from aircraft, towers, and balloon-sondes. Some satellite remote sensing measurements offer additional advantages such as more complete spatial coverage, a vertically-integrated measure of air quality and a measure of long-range transport (e.g., Engel-Cox et al., 2004; Edwards et al., 2006). However, most applications to date have focused on identifying specific events such as forest fires (e.g., Spichtinger et al., 2001) and using satellite retrievals in the context of global-scale air quality modeling (e.g., Shim et al., 2005; Heald et al., 2006; Zhang et al., 2006a). There have been some preliminary applications of using satellite data to study regional air quality such as the use of satellite retrievals to augment the spatial coverage of surface monitoring data (e.g., Liu et al., 2005a) and their assimilation in or comparison with regional air quality model simulations (e.g., Byun et al., 2005; Zhang et al. 2005, 2006b; Pickering et al., 2006; Vijayaraghavan et al., 2006). It is therefore of interest to investigate how satellite measurements can be further used to evaluate regional air quality models.

In this study, we describe the comparison of model predictions from the U.S. EPA Multiscale Air Quality model (CMAQ) for 2001 against tropospheric satellite measurements/retrievals of ozone (O_3) and carbon monoxide (CO).

2. DOMAIN AND MODEL CONFIGURATION

The domain and model configuration used in this study have been described in detail earlier by Zhang et al. (2006b); we present an overview here.

The CMAQ version 4.4 released in October 2004 (Byun and Schere, 2005) is applied to the continental U.S. with a horizontal grid resolution of 36-km. The modeling domain covers the contiguous U.S. and a portion of southern Canada and northern Mexico with 148 × 112 horizontal grid cells. The vertical resolution includes 14 layers from the surface to the tropopause (at ~15 km), with finer resolution in the planetary boundary layer (PBL); the surface layer is 35 m above ground level (AGL).

The meteorological fields, emissions, and initial and boundary conditions for 2001 are provided by the U.S. EPA. The meteorology is driven by the Mesoscale Modeling System Generation 5 (MM5) Version 3.6.1 with four-dimensional data assimilation. The MM5 hourly output files are processed with the Meteorology-Chemistry Interface Processor (MCIP) version 2.2 for CMAQ. The EPA's National Emissions Inventories (NEI) 2001 (also referred to as NEI 1999 Version 3) is used to generate a gridded anthropogenic emission inventory for sulfur dioxide (SO_2), CO, nitric oxide (NO), nitrogen dioxide (NO_2), ammonia (NH_3), volatile organic compounds (VOCs), and particulate matter (PM). The seasonality of the NH_3 emissions is accounted for based on the results of Gilliland et al. (2003) and Pinder et al. (2004). The emission inventory is processed with the Sparse Matrix Operator Kernel Emissions system (SMOKE1.4). A spin-up period of 10 days (December 22-31, 2000) is used to minimize the influence of the initial conditions. The Carbon-Bond Mechanism version IV (CBM-IV) is

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*Corresponding author: Krish Vijayaraghavan, Atmospheric & Environmental Research, Inc., 2682 Bishop Drive, Suite 120, San Ramon, CA 94583; e-mail: krish@aer.com

used for gas-phase chemistry; the default convergence tolerances were tightened to an absolute tolerance of 1×10^{-9} ppm and a relative tolerance of 1×10^{-3} to increase the accuracy in the calculations of fast-reacting radicals such as OH and HO_2. The Regional Acid Deposition Model (RADM) mechanism is used for aqueous-phase chemistry and the CMAQ “aero3” module for aerosol processes.

3. MODEL EVALUATION

The CMAQ model configuration and domain described above were applied for the 2001 calendar year and model output evaluated against satellite retrievals of tropospheric column O_3 and CO vertical profiles.

3.1 Tropospheric Column Ozone

Most techniques used to derive Tropospheric Column Ozone (TCO) from satellite measurements use the tropospheric ozone residual method, wherein TCO is calculated as the difference between Total column Ozone (TO) (mostly from the Total Ozone Monitoring Spectrometer, i.e., TOMS) and Stratospheric Column Ozone (SCO) from other satellite measurements or determined from TOMS data (e.g., Fishman et al., 1987, 2005; Chandra et al., 2003; Ziemke et al., 2006). In all these methods, assumptions are often made about the distribution and variability of SCO.

The first directly retrieved global distribution of tropospheric column ozone from Global Ozone Monitoring Experiment (GOME) measurements was presented by Liu et al. (2005b, 2006a). GOME was launched in 1995 on the European Space Agency’s (ESA’s) second Earth Remote Sensing (ERS-2) satellite to measure backscattered radiance spectra from the Earth’s atmosphere in the wavelength range 240-790 nm (ESA, 1995). Observations with moderate spectral resolution of 0.2-0.4 nm and high signal to noise ratio in the ultraviolet ozone absorption bands make it possible to retrieve the vertical distribution of ozone down through the troposphere (Chance et al., 1991, 1997). The advantage of direct retrievals over the residual-based approaches is that daily global distributions of tropospheric ozone can be derived without other collocated satellite measurements of SCO, or the need to make assumptions about the spatiotemporal distribution of SCO.

In this study, profiles of partial column ozone were retrieved globally from 2001 GOME measurements. The retrieved profiles have 24 layers with the tropopause as one of the levels; the tropopause pressure is based on National Centers for Environmental Prediction (NCEP) /National Center for Atmospheric Research (NCAR) 40-year reanalysis 12 p.m. tropopause pressure. The TCO is the sum of these tropospheric partial columns. GOME observations since 2000 are subject to substantial instrument degradation; an external degradation correction to the radiance and irradiance data was applied to ensure retrieval quality (Liu et al., 2006b).

Three-dimensional (3-D) gridded hourly average O_3 mixing ratios are simulated using CMAQ up to an altitude of about 15 km AGL. The simulated O_3 mixing ratios and MM5-predicted vertically-resolved temperature and pressure are used to calculate the TCO in Dobson units (DUs) as follows:

$$TCO=\sum_{i=1}^{N} (P_i\,\Delta z_i\,A\,[O_3]_{ppm,i}) / (RT_i x 10^6 x C_{DU})$$

where N is the CMAQ layer number corresponding to the tropopause in the GOME TCO retrievals, $[O_3]_{ppm,i}$ is the O_3 mixing ratio in ppm in layer *i*, Δz_i is the height of layer *i* in m, P_i and T_i are the pressure in Pa and temperature in K, respectively, in layer *i*, R is the gas constant (= 8.3145 J $mole^{-1}$ K^{-1}), A is the Avogadro’s number (= 6.02214×10^{23} molecules $mole^{-1}$), and C_{DU} is the conversion factor from molecules O_3 m^{-2} to DU (= 2.68676×10^{22}). Monthly, seasonal, and annual averages are computed for each grid cell. The simulated TCOs are compared with the TCO retrieved from GOME measurements.

3.2 Carbon monoxide

CO mixing ratios simulated with CMAQ are compared with the CO mixing ratios at the following vertical pressure levels (1000 hPa, 850 hPa, 700 hPa, 500 hPa, 350 hPa, 250 hPa, and 150 hPa) derived from the Measurements Of Pollution In The Troposphere (MOPITT) instrument (Edwards et al., 2004) on the NASA Earth Observing System (EOS) Terra spacecraft. The conversion of CMAQ data to the MOPITT vertical grid employed the “vertical averaging” of CMAQ profiles using averaging kernels which represent the manner in which the vertical structure of the atmosphere is mapped into the measured radiances.

4. CONCLUSIONS

Tropospheric column ozone and vertical profiles of carbon monoxide simulated by CMAQ at a 36 km horizontal resolution over the United States were compared to GOME TCO and MOPITT CO retrievals, respectively. Potential reasons for differences include uncertainty in the CMAQ emissions and uncertainties in the GOME retrievals (e.g., due to the limited vertical resolution of the O_3 retrievals, the retrieved profile and TCO are estimates of the actual profile and TCO smoothed by the averaging kernels). While CMAQ model simulations are affected by uncertainties in the model inputs and formulation, satellite retrievals also have limitations such as the effect of clouds (obscuration of the clear-sky path from space to the ground) and the effect of ground albedo (which can result in a lack of contrast between the atmosphere and the surface, making it difficult to obtain the atmospheric quantity from the measurement). However, future generations of satellites (e.g., the polar-orbiting NPOESS sensors and the geostationary GOES-R satellite) will provide enhanced spatial and vertical resolution compared to existing systems.

5. ACKNOWLEDGEMENTS

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