Use of a satellite-based indicator of ozone production sensitivities to diagnose model bias

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Goals: Improving modeled ground-level O_3 predictions

▪Various global/regional chemical transport models (CTMS) including CMAQ model over-predict summer daytime O_3 over the eastern US. For example, over the region, daytime peak O_3 concentrations as predicted by CMAQ model are biased routinely 5-10 ppbv high as compared with surface EPA AQS observations during summer.

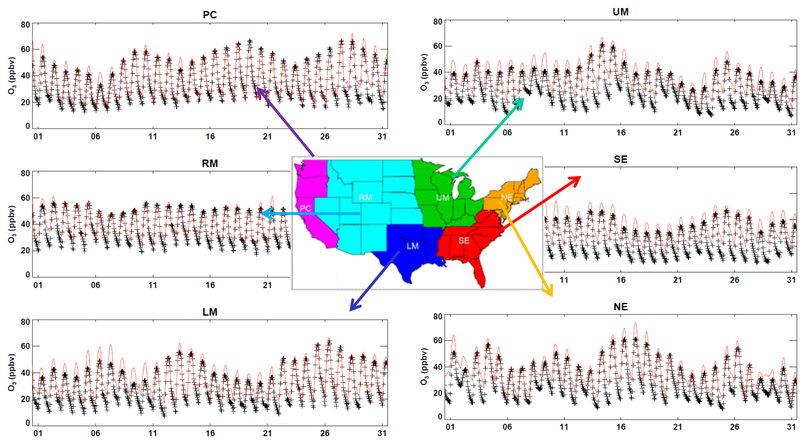

Fig.1 Surface O_3 variation from AQS (black cross line) observations and CMAQ (red solid line) over CONSUS for August 2009

Approaches: the Community Multiscale Air Quality (CMAQ) model version 4.7.1 and satellite resources

1. Model Setup

▪Time period: August 2009 (the greatest O_3 biases from NOAA National Air Quality Forecasting Capability (NAQFC) were shown during 2007 through 2009)
▪Version : CMAQ4.7.1
▪Horizontal and vertical resolution: 12km with 22 vertical layers to 100 hPa
▪Meteorology data: from WRF-NMM
▪Emissions: based on US EPA's NEI 2005
▪CB05(gas-phase chemistry)-AQ(aqueous-phase condition)-AERO5(aerosol chemistry and dynamics) module
▪Boundary chemical condition: GEOS-CHEM simulation

2. Measurements

2.1 Satellite measurement

▪Satellite NO_2 and HCHO column density: from GOME-2 sensor on EUMETSAT MetOp-A satellite
▪GOME-2 NO_2 and HCHO column products are from http://www.temis.nl/airpollution

2.2 In-situ ground measurement

▪Hourly O_3 data: 1100 US EPA's AQS stations

Results:

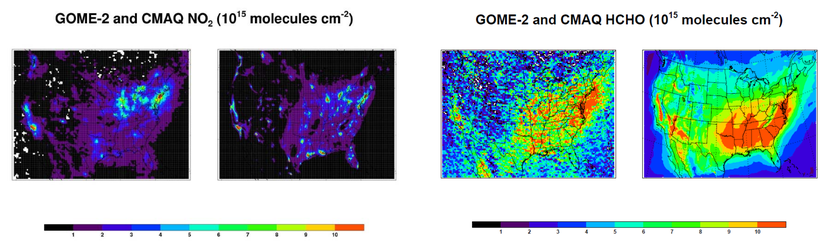

Fig1. Comparison of NO_2 and HCHO columns between GOME-2 and CMAQ4.7.1 (9-10 am, LT) over CONUS for August 2009.

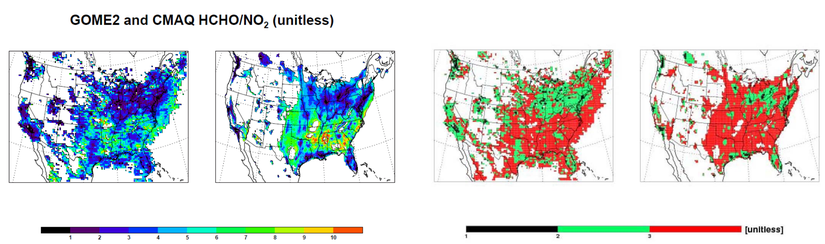

Fig2. Ratio of HCHO to NO_2 between GOME-2 and CMAQ4.7.1 (9-10 am, LT) over CONUS for August 2009. Category 1 (NO_x-saturated regime) is for GOME-2 HCHO/NO_2 < 1, category 2 (mixed regime) is for 1<GOME-2 HCHO/NO_2<3, and category 3 (NO_x-sensitive regime) is for GOME-2 HCHO/NO_2>3.

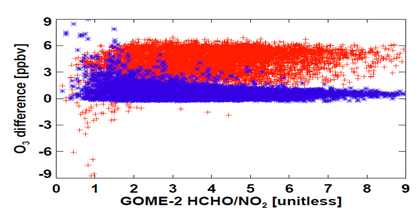

Fig.3 Surface O_3 differences between baseline CMAQ and CMAQ with 30% NO_x (red colored) or VOC emissions (blue colored) reduction according to ratios of GOME-2 HCHO to NO_2 column densities. The difference is estimated by averaging the data for daytime (1-5PM, local time) during August 2009 and are estimated only when GOME-2 NO_2 column density is larger than $1.0x10^{15}$ molecules cm^{-2}.

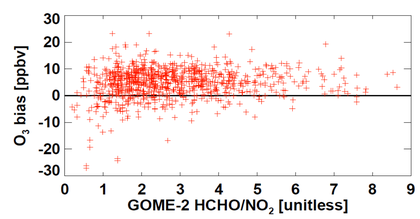

Fig.4 Ozone biases as a function of ratio of GOME-2 HCHO/NO_2 column density for CMAQ baseline simulation. The biases are estimated by averaging differences between daytime (1-5 PM, local time) AQS-measured and CMAQ-simulated O_3 concentrations for August 2009 and are estimated only when GOME NO_2 column density is larger than $1x10^{15}$ molecules cm^{-2} and AQS measurement site exists.

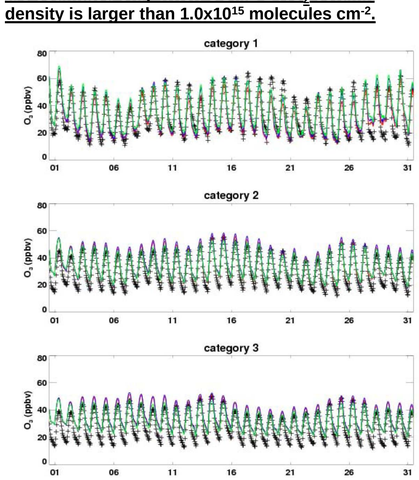

Fig.5 The time series of observed and simulated hourly-averaged O_3 concentrations from AQS (black cross), CMAQ (blue colored), CMAQ with 30% NO_x emissions reduction (green colored), and CMAQ with 30% VOC emissions reduction (red colored) over three GOME-2-derived chemical regimes (NO_x saturated regime, mixed, NO_x-sensitive regime, see Fig. 2) for August 2009.

Results con.:

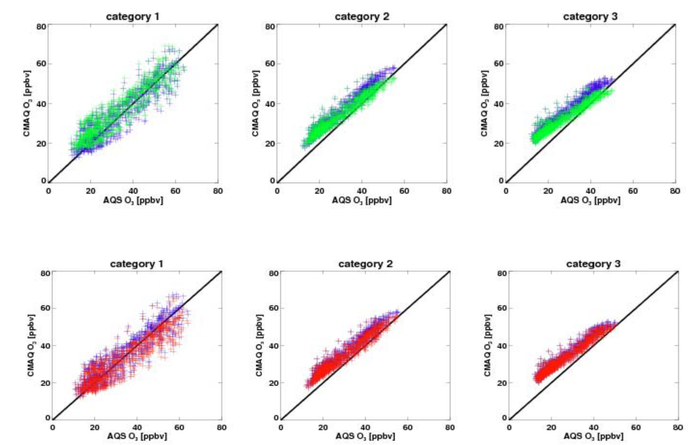

Fig 6. The scatter plots of simulated hourly-averaged surface O_3 concentrations from CMAQ (blue colored), CMAQ with 30% NO_x enmissions reduction (green colored), and CMAQ with 30% VOC emissions reduction (red colored) versus corresponding O_3 concentrations from AQS over three GOME-2 chemical regimes (NO_x-saturated, mixed, NO_x-sensitive regime, see Fig. 2)

Conclusions:

Simulation results from the Community Multiscale Air Quality (CMAQ) model version 4.7.1 over the Conterminous United States (CONUS) for August 2009 are analyzed to evaluate the variation of the hourly-averaged ground-level ozone (O_3) at stations classified according to their O_3-NO_x-VOC chemical sensitivity regimes (Fig. 2). The O_3 sensitivity regimes (NO_x-saturated/mixed/NO_x-sensitive, Fig. 2 & 3) are inferred from the values of photochemical indicators based on the HCHO to NO_2 ratio of column data obtained from the Global Ozone Monitoring Experiment 2 (GOME-2). When compared to the US EPA's Air Quality System (AQS) observations, the CMAQ model over-predicts hourly-averaged O_3 concentrations over the photochemical indicator based regimes (NO_x-saturated: +5.4%, mixed: +22.1%, and NO_x-sensitive:+22.9%, Fig. 4 & 5) with high correlation coefficients. Compared with the base CMAQ run, a 30% NO_x emissions reduction reduces the high O_3 biases over a NO_x-sensitive regime by 7.2%, but it introduces a noticeable worsening in the measured vs. modeled O_3 slope (Fig. 6). This result suggests that future works need to determine the causes of observed modeled O_3 biases in NO_x-sensitive areas.

ACKNOWLEDGEMENTS

This work is dedicated to the memory of Dr. Daewon Byun (1956-2011), whose leadership and pursuit of scientific excellence as the leader of the NOAA Air Resources Laboratory (ARL) Air Quality Group continue to inspire us. We also acknowledge the free use of tropospheric NO_2 and HCHO column data from the GOME-2 sensor from www.temis.nl.

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