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MODELING AND LIDAR STUDY ON OZONE OVER THE CHESAPEAKE BAY DURING OWLETS-2
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ABSTRACT
This study focuses on the distribution of ozone (O3) concentration near the Chesapeake Bay, USA (hereafter CB) by integrating observations and model simulations. The motivation of this work is to understand reasons causing the horizontal and vertical distribution of pollutants (mainly O3) near the CB. The O3 exceedance over the CB happens very frequently during summer and the Maryland Department of Environment intends to find out the reasons in order to make policy-related decision. The observation data used in this study are from the Ozone Water-Land Environmental Transition Study-2 (OWLETS-2) field campaign, including observations from O3 lidar, Doppler wind lidar, ozonesonde. The mesoscale model employed is Weather Research and Forecasting model coupled with chemistry (WRF-Chem) version 3.9.1. The anthropogenic emission dataset is from National Emission Inventory 2011 (NEI-2011), including various emission species, e.g., CO, NOx, SO2, NH3, PM2.5, PM10, etc. The meteorological initial and boundary conditions are from the Northern American Regional Reanalysis (NARR) dataset, which is a high-resolution combined model and assimilated dataset from the National Centers for Environmental Prediction (NCEP). There are several findings of this study based on the model simulations and ground-based observations. Actually, at the beginning of study, we considered two different versions of anthropogenic emissions from NEI-2005 and NEI-2011 developed by the Environment Protection Agency (EPA). EPA added the anthropogenic emissions over CB from boats and ships while updating from NEI-2005 to NEI-2011. For model performance evaluation, we employed AirNow surface hourly O3 mixing ratio diurnal variation and compared it with model simulations.

For instance, at Essex site near Baltimore City, observed O3 has a strong diurnal variation, with minimum (25 ppbv) just after sunrise (05:00 EST), and with maximum (75 ppbv) around afternoon (15:00 EST). Even the model simulation has a good agreement with the observation, it underestimates the mean O3 mixing ratio by about 15-20 ppbv. Both the surface and 700 mb level horizontal spatial distribution of O3 indicate the higher O3 concentration over the north-middle CB, with surface O3 mixing ratio of 40-50 ppbv and 700 mb level O3 mixing ratio of 60 ppbv, which means the surface O3 was lifted up after production. The vertical profiles of wind of both model and Doppler wind lidar match very well, indicating that the model captured the vertical variation of wind. However, the vertical profiles of O3 from model simulation, ozonesonde, and O3 lidar suggests that model simulation underestimated the O3 from surface to 4.5 km. In addition, the model simulation captured the vertical mixing of O3 from surface to 2 km, while misses the O3 variation above 2 km. In order to study the influence of bay breeze on the O3 small scale transport, three vertical cross sections through the CB from west to east at the northern, middle, and southern CB. The results show that higher O3 concentration above the CB. The bay breeze over the southern CB is stronger than the northern CB. The planetary boundary layer height over the CB is dramatically lower than the surrounding land in the day, which contributes to the surface higher O3 concentration over the CB.
1. INTRODUCTION

Tropospheric ozone ($O_3$), especially near the surface, has paramount significant environmental and human health impacts. Long-term exposure to high concentration of $O_3$ can induce serious health issues, for example, irritating lungs, aggravating bronchitis, emphysema and asthma [1-3]. In order to mitigate the surface pollution in the United States, the Clean Air Act requires the Environmental Protection Agency (EPA) to set National Ambient Air Quality Standards (NAAQS). The current NAAQS, in force since 2015, sets an ambient 8-hour $O_3$ mixing ratio criterion of 70 parts per billion by volume (ppbv) (National Ambient Air Quality Standards for Ozone, 2015, hereafter referred to as the Standard; [4]). However, the surface $O_3$ mixing ratio over some specific regions can exceed the Standard, for instance, as in the Chesapeake Bay (hereafter referred to as CB, [5, 6]). All these studies near water bodies surrounded by land and active research are ongoing on understanding the causes for exceedance of $O_3$. As a secondary pollutant, its concentration depends on its precursors, chemical reactions, and meteorological conditions [7, 8]. Understanding these processes helps to understand $O_3$ pollution sources, sinks and is useful for improving the accuracy of $O_3$ pollution forecasting.

As a study to better understand the behavior of $O_3$ and related trace gases across the water land transition $O_3$ in the CB, Ozone Water-Land Environmenal Transition Study (OWLETS) field campaigns (OWLETS-1, 2017 [9]; OWLETS-2, 2018 [10]) integrates ground-based and airborne instruments from multiple institutes. Two key “super-sites” locate at University of Maryland Baltimore County (UMBC) and Hart-Miller Island (HMI) to observe pollutants simultaneously over land and water. All the measurements obtained from OWLETS serve for $O_3$ numerical forecast.

This study further investigates the influence of the CB on the local $O_3$ mixing ratio distribution, by employing a mesoscale model, the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem; [11]). The model performance was evaluated by comparing model output with surface $O_3$ mixing ratio observations. Horizontal and vertical distributions were analyzed by studying the horizontal levels and vertical cross sections through the CB. In terms of novelty, this work utilizes the first-hand ground-based observations from various platforms during OWLETS-2 field campaign, i.e., NASA Goddard Space Flight Center TROpospheric Ozone (TROPOZ) DIAL lidar, NASA Langley Research Center Langley Mobile Ozone Lidar (LMOL), Doppler wind lidar, electrochemical concentration cell (ECC) ozonesonde, and coupled with mesoscale model simulations to study the impact of the CB on the local $O_3$ pollution. Future work includes employing the Data Assimilation Research Testbed (DART, [12]) developed by National Center of Atmospheric Research (NCAR) to assimilate the $O_3$ concentration 3-D distribution by employing both WRF-Chem model and ground-based $O_3$ observations.

2. METHODOLOGY

2.1 Model Configuration

In this study, WRF-Chem version 3.7 is employed to study the influences of CB on the local $O_3$ mixing ratio distribution in 3-D, along with the interaction between $O_3$ mixing ratio and meteorological fields. WRF-Chem is a fully coupled “online” model, which has the air quality component consistent with the meteorological components [11]. The gas-phase chemistry and aerosol module are based on the Carbon-Bond Mechanism Version Z (CBM-Z, [13]) and Model for Simulating Aerosol Interactions & Chemistry (MOASIC, [14]). Radiation treatment utilizes the RRTMG short-wave and long-wave radiation schemes [15], without including the aerosol feedback. The radiation scheme setups are recommended for the model simulations over the continental U.S. by the WRF team [16].

The model study area (Fig. 3.1) is set up to start with the eastern U.S. The outer domain is further resolved by one two-way nested grid region that progressively focuses and centers on the study region, the CB. Thus, two domains are established, an outer domain (spatial resolution of $9 \times 9$ km, d01) and a nested domain ($3 \times 3$ km, d02), selected for concentrating on detailed $O_3$ concentration and evolution investigation. Along the vertical, 35 levels are used with the model top located at 100 hPa and about 10-15 of the vertical levels set
below 800 hPa, in order to resolve the planetary boundary layer (PBL). While there are several PBL schemes, the YSU scheme [17, 18] was selected for the runs shown here based on the performance evaluation through previous studies [19].

In addition, EPA updated anthropogenic emissions over the CB when comparing NEI-2005 and NEI-2011 (Fig. 3.2). Several emission species were added over the CB, e.g., CO, NOx, SO2, NH3, PM2.5, PM10.

![Model domain setup with 9 km (red rectangle) outer domain and 3 km nested domain (pink rectangle).](image1)

**Fig. 3.1** Model domain setup with 9 km (red rectangle) outer domain and 3 km nested domain (pink rectangle).

**2.2 TROPOZ and LMOL ozone lidar**

The NASA Goddard Space Flight Center TROPOZ DIAL lidar has been developed in a transportable trailer and used to take measurements of tropospheric ozone at UMBC (38.99N, 76.84W) [21]. The NASA Langley Research Center developed LMOL lidar and used to take measurements at HMI (39.24N, 76.36W) [22]. They are a part of the ground-based Tropospheric Ozone Lidar Network (TOLNet, https://wwwair.larc.nasa.gov/missions/TOLNet/index.html) which is designated to improve the current number of tropospheric ozone profiles [20]. TOLNet is a network of ozone lidar stations across the U.S. and Canada with the objective of improving the tropospheric O3 vertical profile observation. Currently, TOLNet has seven stations and is designed to provide regular, high fidelity measurements of O3 within the troposphere particularly the changing O3 dynamics and laminiae inside the PBL. We used the data observed by the GSFC TROPOZ DIAL lidar and LaRC LMOL lidar to evaluate the model performance on the O3 vertical profile in this study.

**3. RESULTS**

**3.1 O3 Diurnal Variation**

Surface O3 diurnal variations from both AirNow surface observations and WRF-Chem simulations on June 29, 2018 are shown in Fig. 3.3. The observed O3 has a strong diurnal variation, with minimum (25 ppbv) just after sunrise, and maximum (75 ppbv) around afternoon. This is due to the large emissions during daytime and O3 precursor photochemical reactions. Nevertheless, simulated O3 also has similar diurnal variation as observation, albeit with significant underestimates about 15-20 ppbv. The explanation to this is that we did not include biogenic emissions in the model simulation.

![Diurnal variation of O3 mixing ratio at the surface from EPA AirNow and WRF-Chem simulation from two AirNow sites in Maryland (Essex and Calvert). The red shaded areas are standard deviations. O3 surface mixing ratio daily averages are denoted as dashed lines, with blue for AirNow and red for WRF-Chem.](image2)

**Fig. 3.3** Diurnal variation of O3 mixing ratio at the surface from EPA AirNow and WRF-Chem simulation from two AirNow sites in Maryland (Essex and Calvert). The red shaded areas are standard deviations. O3 surface mixing ratio daily averages are denoted as dashed lines, with blue for AirNow and red for WRF-Chem.

**3.2 O3 Vertical Profile**

**3.2.1 Ozonesonde**

The O3 vertical profiles from both ozonesonde and model simulation are shown in Fig 3.4. At UMBC, observed O3 vertical profile from ascending (blue) has finer vertical resolution, with O3 well-mixed below 2.5 km. Simulated O3 captures this well mixture near the surface, but misses the trend above 2.5 km. At HMI, the observed O3 increases rapidly from 60 to 85 ppbv from surface to 200 m. Note that the descending ozonesonde profile could be very far away from the original launch location, and the observation time could be hours later after launch.
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REFERENCES