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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, NO_x, SO₂, NH₃, PM_{2.5}, 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 . 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 Environmental 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 (MOSAIC, [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 9×9 km, d01) and a nested domain (3×3 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].



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

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, NO_x, SO₂, NH₃, PM_{2.5}, PM₁₀.

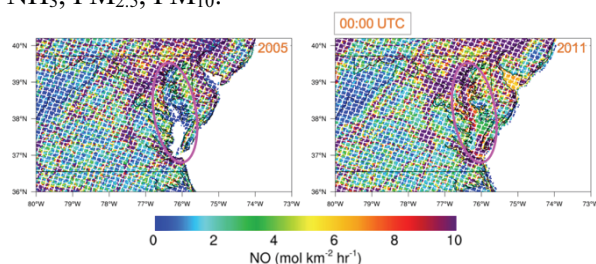


Fig. 3.2 NO emissions from NEI-2005 (left) and NEI-2011 (right). The pink ellipse shows NO emissions over the CB.

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 laminae 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 with 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.

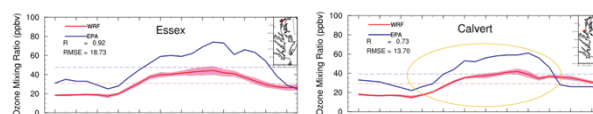


Fig. 3.3 Diurnal variation of O₃ mixing ratio at the surface from EPA AirNow and WRF-Chem simulation from two AirNow sites in Maryland (Essex and Calvert). The red shaded areas are standard deviations. O₃ surface mixing ratio daily averages are denoted as dashed lines, with blue for AirNow and red for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

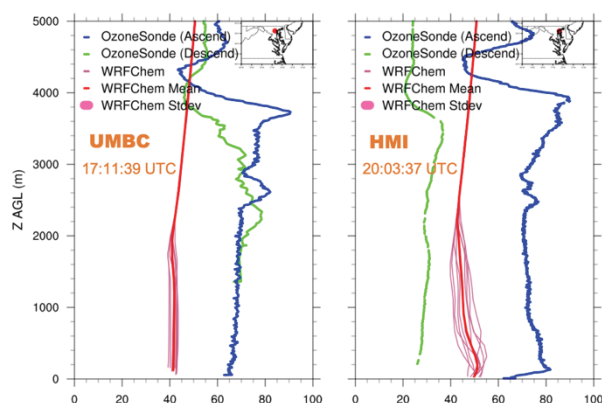


Fig. 3.4 O₃ vertical profiles from ozonesonde at UMBC (launch time at 17:11:39 UTC) and HMI (launch time at 20:03:37 UTC) sites on June 29, 2018. Blue is ascending, green is descending, and red is model simulation.

3.2.1 TROPOZ and LMOL O₃ lidar

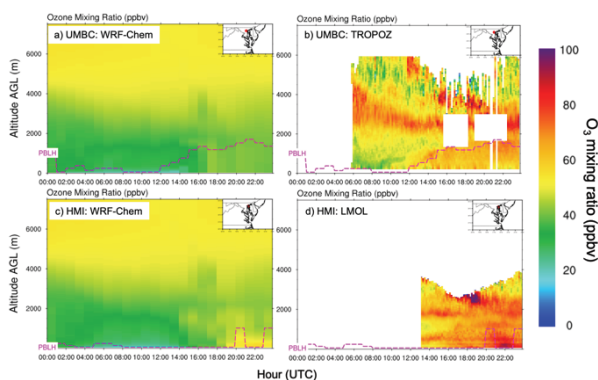


Fig. 3.5 O₃ vertical profile time series on June 29, 2018 observed by TROPOZ O₃ lidar at UMBC (b) and LMOL O₃ lidar at HMI (d). The corresponding model simulated O₃ vertical profile time series are shown in (a) and (c), respectively. PBLH from model simulation is denoted by pink curve.

From the O₃ vertical profile diurnal variation (Fig. 3.5), near-surface O₃ mixture is significantly influenced by the variation of the planetary boundary layer height (PBLH). As PBLH is shallow at night, there is lower O₃ to the surface. While PBLH increases in the day, O₃ is mixed down to the surface and well-mixed within 2 km. At UMBC, there are two layers with higher O₃ concentration from 2-4 km (Fig. 3.5 b). While at HMI, higher O₃ concentration was found near the CB surface (Fig. 3.5 d). The contribution of high O₃ concentration might be transported from long-range transport. In addition, PBLH fluctuates at HMI around 22:00 UTC. More evidence is needed to confirm it.

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REFERENCES

- [1] M. Lippmann, Environmental Science & Technology. 25, 1954-1962 (1991)
- [2] I. S. Mudway & F. J. Kelly, Molecular aspects of medicine, 21(1-2), 1-48 (2000)
- [3] M. H. Forouzanfar. et al. The Lancet, 388(10053), 1659-1724 (2016)
- [4] O. R. Cooper, Science, 348(6239), 1096-1097 (2015)
- [5] C. P. Loughner, Journal of Applied Meteorology and Climatology, 53(7), 1697-1713 (2014)
- [6] J. T. Sullivan, Bulletin of the American Meteorological Society, 100(2), 291-306 (2019)
- [7] U. PROG, United Kingdom Photochemical Oxidants Review Group Report, Department of the Environment, London (1997)
- [8] M. E. Jenkin, & K. C. Clemitshaw, Atmospheric Environment, 34(16), 2499-2527 (2000)
- [9] J. T. Sullivan, et al., Bulletin of the American Meteorological Society, 100(2), 291-306 (2019)
- [10] J. T. Sullivan, T. Berkoff, J. Dreessen, R. Delgado, G. Gronoff, L. Nino, B. Carroll et al. In AGU Fall Meeting Abstracts. 2018.
- [11] G. A. Grell, et al., Atmospheric Environment, 39: 6957-6975 (2005)
- [12] J. Anderson et al., Bulletin of the American Meteorological Society, 90(9), 1283-1296 (2009)
- [13] R. A. Zaveri and L. K. Peters, J. Geophys. Res., 104, 30387-30415 (1999)
- [14] R. A. Zaveri, et al., J. Geophys. Res., 113, D13204, doi:10.1029/2007JD 008782 (2008)
- [15] M. J. Iacono, et al., J. Geophys. Res., 113, D13103, doi:10.1029/2008JD-009944 (2008)
- [16] S. E. Peckham, WRF/Chem version 3.9 user's guide (2017)
- [17] S. Y. Hong and H. L. Pan, Mon. Weather Rev. 124: 2322-2339 (1996)
- [18] S. Y. Hong, et al., Mon. Weather Rev. 134: 2318-2341 (2006)
- [19] X. Hu, et al., Journal of Applied Meteorology and Climatology, 49(9), 1831-1844 (2010)
- [20] T. Leblanc, et al., Atmospheric measurement techniques, 11, 6137-6162 (2018)
- [21] J. T. Sullivan, T. J. McGee, G. K. Sumnicht, L. W. Twigg, and R. M. Hoff., Atmospheric Measurement Techniques, 7(10):3529-3548, (2014)
- [22] R. De Young, Carrion, W., Ganoe, R., Pliutau, D., Gronoff, G., Berkoff, T., & Kuang, S., Applied optics, 56(3), 721-730. (2017)