THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY

Sources of secondary organic aerosols in the Pearl River Delta region: contribution from the oxidation of semi-volatile primary organic aerosols

Teng Yao[1], Jimmy C.H. Fung[1, 2], Siyuan Wang[3], YongJie Li[1], Jian Zhen Yu[1, 3], Chak K. Chan[1, 4], Alexis K.H. Lau[1, 5]

[1]Division of Environment, The Hong Kong University of Science and Technology, Hong Kong
[2]Department of Mathematics, The Hong Kong University of Science and Technology, Hong Kong
[3]Department of Chemistry, The Hong Kong University of Science and Technology, Hong Kong
[4]Department of Chemical and Biomolecular Engineering, Hong Kong University of Science and Technology, Kowloon, Hong Kong.
[5]Department of Civil and Environmental Engineering, The Hong Kong University of Science and Technology, Hong Kong

Objective

- To evaluate the SOA formation from the oxidation of semi-volatile POA with the Volatility Basis-Set (VBS) model.
- To improve air quality forecast via augmenting new model modules.

Introduction

1. Serious particulate pollution in the Pearl River Delta region

As China's largest economic development zone, the Pearl River Delta region (PRD, location shown in Figure 1) suffers from particulate matter (PM) pollution. Haze days due to high PM concentration, have occurred frequently in this region. Besides deterioration of visibility, PM pollution also causes a negative impact on residential health. It is also report that in PRD region, PM abundance is associated with the mortality of lung cancer. In a later study on the health impact of air pollution, it is identified that in the PRD region exposure to PM and gaseous pollutants causes adverse effect on lung function growth in schoolchild. Recent studies underscore the need to improve our understanding of the PM pollution of the PRD region.

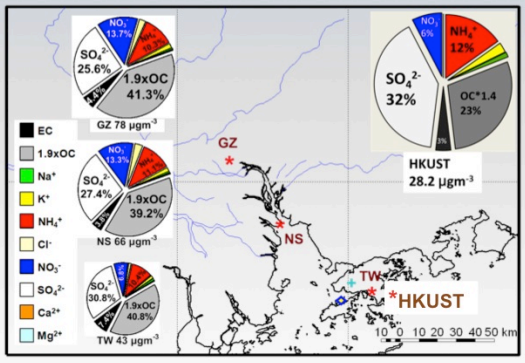

Figure 1. Observed $PM_{2.5}$ concentration shows PRD is suffering from a serious PM pollution problem with annual average of $PM_{2.5}$ concentration spanning from 28 to 78 ug/m^3 (Huang et al., 2013).

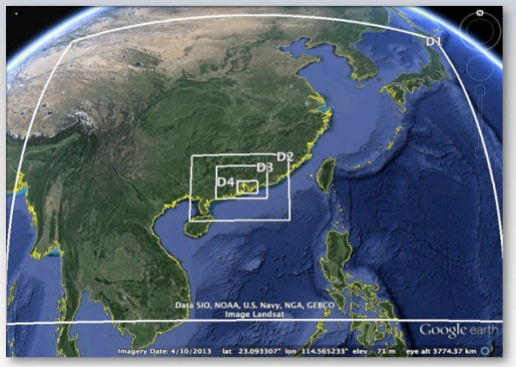

Figure 2. To study PM pollution in the PRD, WRF and CAMx applies D1-D2-D3-D4 (27k-9km-3km-1km) simulation domains zooming down from Asia to PRD.

2. under-estimation of secondary organic aerosol

WRF (version 3.6) and CAMx (version 5.41) simulation are carried out to study the PRD's PM pollution, and simulation results (Figure 3 and 4) show one of PM's major components, secondary organic aerosol (SOA) is constantly under-estimated.

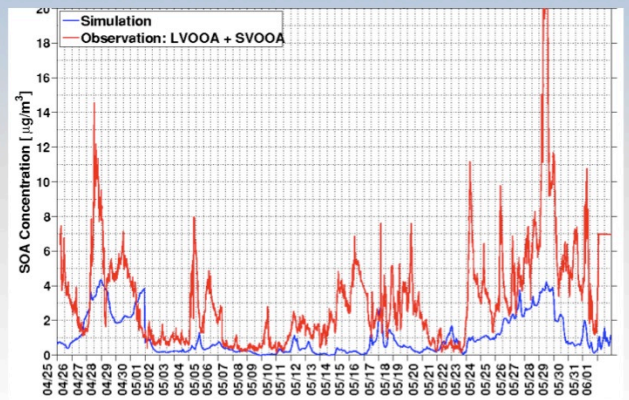

Figure 3. Comparison between simulated and AMS observed SOA concentration over HKUST during April-May, 2011.

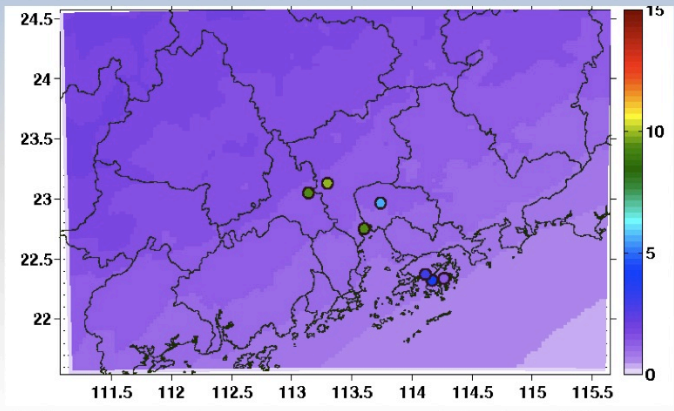

Figure 4. Comparison between annual average of simulated SOA concentration and observed SOA concentration (small circles, obtained via ECOC tracer method) shows SOA is largely under-estimated.

Methodology

Implement of Volatile Basis Set Model

In this study, the POA from diesel engine exhaust, gasoline engine exhaust, and biomass burning emission are distributed into 9 lumped species based on the method introduced by Grieshop et al. (2009). Lumped species are involved in oxidization reaction with OH radical. The oxidizing mechanism is constituted with two-bin-shift generation of oxidation, and the OH reaction rate is 2×10^{-11} cm^3 $mole^{-1}s^{-1}$. During the reactions, the organic mass is increased by 40% for each generation of oxidation (equivalent to adding about 5 oxygen atoms to C15 alkane).

Result

1. Improved SOA simulation

After VBS model implemented into CAMx, the simulated trends and level of concentration of SOA are improved. Figure 5 shows the observed and simulated time series of SOA concentration over HKUST during April-May, 2011, and Figure 6 provides annual average of SOA concentration simulated via CAMx with VBS. It can be seen that the CAMx continuously under-estimates the SOA concentration; on the other hand, the updated CAMx with VBS, could provide a more reasonable SOA concentration level, and a rather consistent variation with observed SOA concentration.

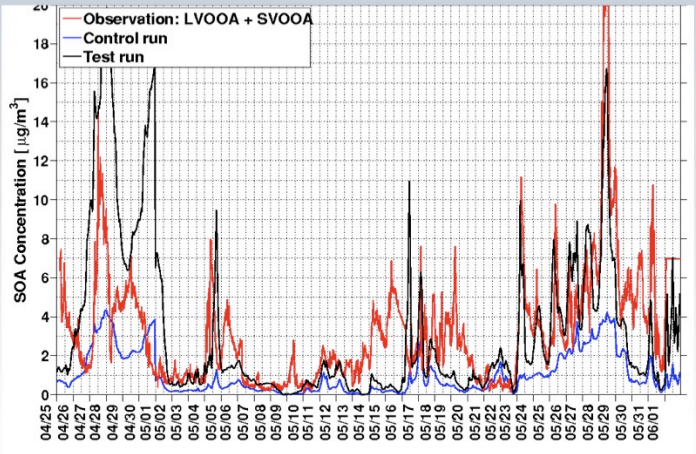

Figure 5. Comparison among control run (CAMx untouched), test run (CAMx with VBS), and AMS observed SOA concentration over HKUST during April-May, 2011.

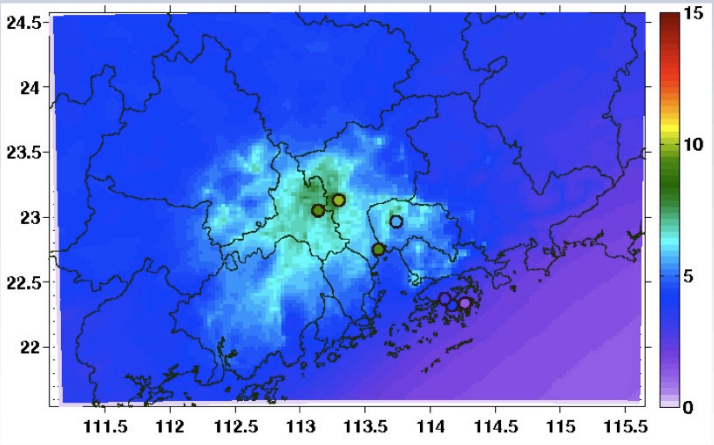

Figure 6 shows annual average of simulated SOA concentration based on CAMx with VBS. Small circles refer to observed SOA concentration (obtained via ECOC tracer method).

2. Evaluation of SOA production from oxidation of POA

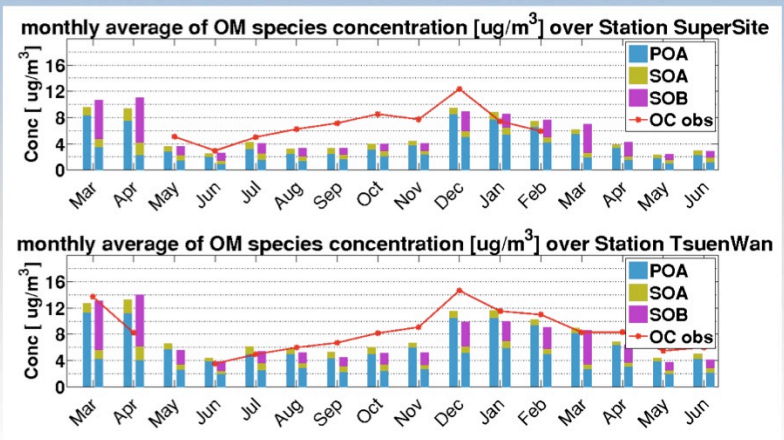

Figure 7 shows monthly average of simulated organic aerosol concentration from control run (CAMx untouched, bars on the left of each pair), and test run (CAMx with VBS, bars on the right of each pair). Pink tabs (SOB) refer to the product from oxidation of volatile POA. It can be seen that oxidation of POA contributes around 2-7 ug/m³ SOA in the PRD.

Although organic matter gains weight during oxidation, the total concentration of organic matter in test run is lower than control run, since after VBS module assigns POA from diesel engine exhaust, gasoline engine exhaust, and biomass burning into both gas-phase and particle-phase, there is still volatile POA floating in the air.

Conclusion

With VBS model implemented into CAMx, simulation result shows that CAMx with VBS model provides a better SOA simulation compared with the CAMx with nonvolatile POA emission, which predicts the average SOA concentration around 2 ug/m³ over the PRD, under-estimating by 2-7 ug/m³ (around 60% - 90% of the observed SOA concentration). After the implementation, simulation result shows that CAMx with VBS model provides a more realistic SOA concentration level, and temporal variations of SOA concentration with better agreement with the observation.

Reference

Grieshop, A.P., Logue, J.M., Donahue, N.M., and Robinson, A.L. (2009) Laboratory investigation of photochemical oxidation of organic aerosol from wood fires 1: measurement and simulation of organic aerosol evolution, Atmos. Chem. Phys., 9, 1263–1277.

Huang, X. H., Bian, Q., Ng, W. M., Louie, P. K., & Yu, J. Z. (2013). Characterization of PM 2.5 Major Components and Source Investigation in Suburban Hong Kong: A One Year Monitoring Study. *Aerosol and Air Quality Research, under preparation*.