Student/ Group - First Name, Surname

Small-Scale Research Project (SSRP) – Exercise

Physical and chemical model study on the formation and growth of secondary organic aerosols (SOA)

Teacher: Michael Boy

Model: MALTE-Box

20-25 April 2020
St. Petersburg, Russia

Russian State Hydrometeorological University (RSHU)

EXERCISE – Small-Scale Research Project (SSRP): General Information

Physical and chemical model study on the formation and growth of secondary organic aerosols (SOA)

Model used: **MATLE-Box**

Teacher: **Michael Boy**

Introduction Background (Xavier et al., 2019):
Atmospheric secondary organic aerosols, formed from gas- to particle phase conversion of the oxidation products of volatile organic compounds (VOCs), significantly impact the organic aerosol mass loadings. However, the scale of SOA contribution to the aerosol particle mass is still subject to high uncertainties. The elevated aerosol particle concentrations are shown to have inimical effects on health and a varying degree of influence on the climate by forming cloud condensation nuclei (CCN), altering the cloud properties and radiative balance. Therefore, it is acutely necessary to understand the contributions and role of SOA in the particle loading in the atmosphere. Biogenic VOCs from forest are estimated to contribute to about 90% of VOC emissions globally. The most important BVOCs for SOA formation are isoprene (C_5H_8), monoterpenes ($C_{10}H_{16}$) and sesquiterpenes ($C_{15}H_{24}$). These compounds are all alkenes containing at least one carbon–carbon double bond, enabling them to undergo oxidation by the dominant atmospheric oxidants: the hydroxyl radical (OH), ozone (O_3) and the nitrate radical (NO_3). For some of the terpenes, initial oxidation steps can lead to formation of highly oxygenated organic molecules (HOMs). Some of these HOMs generally have low volatilities and can condense nearly irreversibly, thereby producing SOA.

Main Goal:
In this SSRP you will apply the model MALTE-Box to investigate the formation rate of clusters by varying the main parameters (e.g. sulphuric acid, ammonia, condensation sink, temperature). Further you will investigate the growth of these clusters by low volatile organic compounds by applying the new peroxy radical autoxidation mechanism (PRAM) to model the concentrations of highly oxygenated organic molecules (HOM) from the precursors (e.g. terpenes).

Specific Objectives:
1. Get information on the concentrations of the most important precursors (in MALTE-Box they are NH_3, SO_2/H_2SO_4 and background particle concentration) of cluster formation. Assume that these concentrations vary within one or two orders of magnitude (or whatever is realistic) and examine the impact on particle formation.
2. Based on your cluster formation rate you will then study the growth of the new formed particles by semi-, low and extreme low volatile organic compounds. Therefor you will use the chemistry from the Master Chemical Mechanism (MCM) and the new developed PRAM with various concentrations for the precursor compounds. The simulations will provide you detailed particle composition in time, size and chemical species, which you will analyze to understand the main drivers in the SOA growth mechanism.
3. Visualize your findings in a condensed way by applying your own plotting software and discuss how your outcome in a convincing way relates to initial conditions and other parameters. How localized sources like animal husbandry or change in land-use is impacting your results.

Literature List:

Before the course, you should read, at least, the following three publications; other papers on this topic are recommended to read and will be useful for the discussions/talks (but not obligatory).

REQUIRED READINGS

Roldin, P., Ehn, M., Kurtén, T., Olenius, T., Rissanen, M. P., Sarnela, N., Elm, J., Rantala, P., Hao, L., Hyttinen, N., Heikkinen, L., Worsnop, D. R., Pichelstorfer, L., Xavier, C., Clusius, P., Öström, E., Petäjä, T., Kulmala, M., Vehkamäki, H., Virtanen, A., Riipinen, I., and Boy, M.: The role of highly oxygenated organic molecules in the Boreal aerosol-cloud-climate system, Nature Communication, 10, 4370, doi.org/10.1038/s41467-019-12338-8, 2019

Xavier, C., Rusanen, A., Zhou, P., Dean, C., Pichelstorfer, L., Roldin, P., and Boy, M.: Aerosol mass yields of selected biogenic volatile organic compounds – a theoretical study with nearly explicit gas-phase chemistry, Atmos. Chem. Phys., 19, 13741–13758, https://doi.org/10.5194/acp-19-13741-2019, 2019

Qi, X., Ding, A., Roldin, P., Xu, Z., Zhou, Z., Sarnela, N., Nie, W., Huang, X., Rusanen, A., Ehn, M., Rissanen, M. P., Petäjä, T., Kulmala, M. and Boy, M.: Modelling studies of HOMs and their contributions to new particle formation and growth: comparison of boreal forest in Finland and a polluted environment in China, Atmos. Chem. Phys., 18, 11779-11791, 2018

Schedule for the Research Training – Small-Scale Research Projects/ Exercises

Day	Period	Total time	Topics to be discussed	Runs	Comments	Assistance
(1) Monday	13:30-18:00+	4 h +	General information provided for MALTE-Box and the chemical and physical background of the model Literature research for precursors + ***INDEPENDENT WORK***	On your own laptop	Lecturing Check literature and databases Select parameters for the runs Test runs on computer Discussion on the plan of the SSRP	Teacher
(2) Tuesday	13:30-18:00+	4 h +	Lecture for applying MALTE-Box – the new GUI interface Model simulations in two groups + ***INDEPENDENT WORK***	On your own laptop	Lecturing Test & continue runs on computer Start visualization Start analysis Discussion on the plan of the SSRP	Teacher
(3) Wednesday	13:30-18:00+	4 h +	Model simulations in two groups Analyses of modelling results Discussion with the whole SSRP group on the intermediate results + ***INDEPENDENT WORK***	On your own laptop	Students present project outline/tasks Continue runs on computer Continue visualization Continue analysis	Teacher
(4) Thursday	13:30-18:00+	4 h +	Model simulations in two groups Analyses of modelling results Discussion with the whole SSRP group on the intermediate results + ***INDEPENDENT WORK***	On your own laptop	Finish runs on computer Continue visualization Continue analysis Draft presentation	Teacher
(5) Friday	13:30-18:00+	4 h +	Model simulations in two groups Analyses of modelling results Discussion with the whole SSRP group on the intermediate results + ***INDEPENDENT WORK*** Oral presentation preparation		Finalize analysis Finalize presentation Students practice pres. results	Teacher
(6) Saturday	08:30-09:15+ 09:20-12:00+	4 h +	Final practicing on presentation Oral presentation	Defence of small-scale research project (SSRP) Awarding diploma/ certificates		