

SIMULATION OF THE EFFECTS OF LOW VOLATILITY ORGANIC COMPOUNDS ON AEROSOL NUMBER CONCENTRATIONS IN EUROPE

David Patoulias^{1,2,*} and Spyros N. Pandis^{1,2}

^[1] Department of Chemical Engineering, University of Patras, Patras, Greece

^[2] Institute of Chemical Engineering Sciences, Foundation for Research and Technology – Hellas
(FORTH/ICE-HT), Patras, Greece

* [Email: davidpat@chemeng.upatras.gr](mailto:davidpat@chemeng.upatras.gr)

ABSTRACT

A three-dimensional chemical transport model (PMCAMx-UF) is used to simulate the size distribution and composition of ultrafine particles^[1]. In this work, the model is extended with the addition of chemical aging reactions of semi-volatile organic compounds (SVOCs), the emissions and chemical aging of intermediate volatile organic compounds (IVOCs) and the production of extremely low volatility organic compounds (ELVOCs) monoterpenes. For the simulation of aerosol microphysics, PMCAMx-UF uses the updated version of DMANx which simulates the processes of coagulation, condensation/ evaporation and nucleation with the two-moment aerosol sectional (TOMAS) algorithm^[2]. The model is applied in Europe to quantify the effect of these processes on particle number concentrations. The model predictions are evaluated against both ground measurements collected during the PEGASOS 2012 campaign in several stations in Europe and airborne observations by a Zeppelin measuring above Po-Valley (Italy). PMCAMx-UF reproduced the ground-level daily average concentrations of particles with diameter larger than 100 nm (N_{100}) with normalized mean error (NME) of 45% and normalized mean bias (NMB) close to 10%. For the same simulation, PMCAMx-UF tends to overestimate the concentration of particles with diameter larger than 10 nm (N_{10}) with a daily NMB of 23% and a daily NME of 63%. The model was able to reproduce more than 75% of the N_{10} and N_{100} airborne observations (Zeppelin) within a factor of 2.

KEYWORDS: PMCAMx-UF, Modeling, Air pollution, Nucleation, Aerosol number concentration

REFERENCES

[1] Patoulias, D. and Pandis, S. N. (2022). Simulation of the effects of low-volatility organic compounds on aerosol number concentrations in Europe, *Atmos. Chem. Phys.* 22 (3), 1689–1706.

[2] Adams, P. J. and Seinfeld, J. H. (2002) Predicting global aerosol size distributions in general circulation models, *J. Geophys. Res.* 107 (D19): 4370.