Atmospheric Chemistry and Physics Discussions

Atmos. Chem. Phys. Discuss., author comment AC2
https://doi.org/10.5194/acp-2021-655-AC2, 2021

Reply to the Comments of Referee #2

David Patoulias and Spyros N. Pandis

Author comment on "Simulation of the effects of low-volatility organic compounds on aerosol number concentrations in Europe" by David Patoulias and Spyros N. Pandis, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2021-655-AC2, 2021

---

(1) *The manuscript "Simulation of the effects of low volatility organic compounds of aerosol number concentrations in Europe" by Patoulias and Pandis presents a model investigation on how including extremely low volatile organic compounds and intermediate volatility organic compounds affect simulated aerosol number (and mass) concentrations. The manuscript is very well written and the topic of the paper addresses relevant scientific questions within the scope of Atmospheric Chemistry and Physics. There are few models around that can simulate the formation and growth of aerosol by gas-to-particle partitioning of semivolatile organic compounds as detailed as PMCAMx-UF. Although the results indicate that these compounds have a minor effect on aerosol number concentrations over the studied region, it is an interesting result. I recommend publishing this manuscript once the following minor points have been addressed.*

We thank the reviewer for the positive assessment of our study. We do agree that the main result of our paper is rather surprising. Our responses to the comments of the reviewer and the corresponding changes to the paper (in regular font) follow each comment of the reviewer (in italics).

(2) *In the model description, it is laborious to piece together the methods that the model uses for aerosol physics since the description relies on referenced articles. For example, solving condensation of inorganic and organic compounds simultaneously remains unclear to me. It seems that organics are always assumed to be in a separate phase from water and inorganics. Is this correct? In addition, it seems that water uptake uses a parameterization for bisulfate. Is the amount of sulfate equal to the amount of bisulfate in particles? Are organic compounds assumed to be hydrophobic?*

We have added information to the model description section addressing the main points raised by the reviewer. Indeed, the model assumes that organics and inorganics are in different phases, but in the same particles. Therefore, the condensation of one affects the size distribution of the particles and therefore the condensation rate of the other. The inorganic aerosol thermodynamics including the sulfate/bisulfate split and the water uptake by all inorganic aerosol components are simulated with a detailed aerosol thermodynamics model, ISORROPIA. The water content of the organic aerosol is neglected in this version of PMCAMx-UF and the aerosol water is dominated by the inorganic aerosol components. Additional information can be found in previous publications describing the

evolution of PMCAMx-UF (Jung et al. 2010; Fountoukis et al. 2012; Patoulias et al. 2018).

(3) *It would also be helpful for the reader to summarize the ELVOC yields and IVOC emissions in a table.*

We have followed the suggestion of the reviewer and moved Table S1 from the supplementary material to the main text. This was also recommended by reviewer 1 (comment 2). We have made changes in the main text, clarifying the emissions/yields used in each simulation.

(4) *Line 174: Murphy at al. => Murphy et al.*

We have corrected the typo.

(5) *Line 183: Are IVOCs additional to POA?*

IVOCs were not included in the original emission inventory and therefore have been added to the emissions. Their emission rate is scaled based on the non-volatile POA emissions included in the inventory. Their total emission rate is assumed to be 1.5 times the non-volatile POA emissions. This is now explained in the revised paper.

(6) *Is modelled OA in $PM_{2.5}$ and filter measured OA in $PM_{2.5}$ fully comparable as part of semivolatile compounds in filter samples can be evaporated, while modelled OA will include all semivolatile material?*

The measurement of OA using filters is characterized by two artifacts: a positive one involving adsorption of organic vapors on the quartz filters used for the sampling and a negative one related to the evaporation of some of the semi-volatile material. There is a rich literature on the magnitude of these artifacts and on ways to minimize them or correct for them (involving denuders for removal of organic vapors and after-filters). In this work, we use the reported measurements for the model evaluation keeping in mind their uncertainty. A brief discussion of this point has been added to the paper.

(7) *In Conclusions Lines 485-489 it is said that the growth of the newly formed particles is suppressed because changes in size distribution decrease nucleation rates, sulfuric acid concentrations, and increase the coagulation sink. However, these changes are not backed up with numbers. This conclusion is probably true, but needs to be diagnosed from the model.*

We have followed the suggestion of the reviewer and prepared a new figure (included in the supplementary information) showing the fractional change in the number concentration of $N_{1\text{-}10}$ (reflecting nucleation rates), sulfuric acid, condensational sink and coagulation sink due to the ELVOCs. This figure supports quantitatively our argument of decreasing nucleation rates, decreasing sulfuric acid levels and increasing coagulation/condensational sinks when ELVOCs are added to the model. These changes are especially pronounced in the Scandinavian Peninsula.