Geoscientific

Model Development

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Discussions

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comment

Interactive comment on "ORACLE 2-D (v2.0): An efficient module to compute the volatility and oxygen content of organic aerosol with a global chemistry – climate model" *by* Alexandra P. Tsimpidi et al.

Anonymous Referee #1

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The manuscript describes and evaluates a module for simulating organic aerosol, its volatility, and the oxidation state in a global model framework. The module is one of the most advanced available for global scale atmospheric models and thus the manuscript is well within the scope of Geoscientific Model Development. The manuscript is for the most part well written. However, some parts which are detailed below need clarification and correcting. I can recommend publishing the manuscript after the following issues have been considered:

- The treatment of POA is unclear to me. Do you assume some volatility distribution for it? According to Page 13 this seems to be the case as it is said that it evaporates due to dilution (Line 340). What O:C ratio or O:C ratio distribution is assumed for POA?

- What is assumed for the size distribution of OA which partitions from gas to particles? Does it follow the modal approach presented in Tsimpidi et al., 2014?

- Page 9: All the abbreviations of organic aerosol species are not explained in this paper, i.e. aSOA-v, bSOA-v, SOA-sv, SOA-iv

- Page 10, Section 3.5: After reading this section it is still not obvious to me how gas-particle partitioning is actually calculated. Does $C_{a,i}$ in Equations (11) and (12) correspond to $\sum_{j=1}^{m} \text{SOA}_{i,j}(t + \Delta t)$ in Equation (14)? If so, is it also correct that Equation (11) is first solved for one volatility bin and then the total concentration in that bin is divided among the O:C bins using Equations (13) and (14) based on the O:C distribution on the previous time step? Do you use mole fraction from the previous time step for all the volatility bins? This procedure should be explained in more detail.

- In Equation (11) it is assumed that the saturation ratio at the particle surface is dependent on the mole fraction of compounds in the organic phase. This is a common practice when solving SOA partitioning, but how good is this assumption in the atmosphere? In many cases, especially at the top of the boundary layer, humidity can be so high that the majority of moles in the aerosol is water decreasing significantly the mole fraction of individual SOA species compared to when only organic phase is taken into account. Thus SOA formation is underestimated. Can you comment on this?

- The model is evaluated with observations only at the ground level. However, accounting for the volatility has implications on the vertical profiles of OA and as

there are aircraft campaigns where OA has been measured with aerosol mass spectrometers, it would be interesting how well the model compares with the observations in the vertical.

- Can you give some estimate on the increase in the computation time when moving from the 1-D ORACLE to 2-D ORACLE?

Technical comments and typos:

- Page 2, Line 36: space missing before the word "Organic"

- Page 3, Line 44: pas-aerosol → gas-aerosol

- Page 10, Line 270: equation → equations

- Figure 1a: Compustion → Combustion

- Figure 8 caption: To be consistent with the rest of the manuscript, please change SV-OOA → SVOOA and LV-OOA → LVOOA