

Advanced modeling of gas chemistry and aerosol dynamics with SSH-aerosol v2.0

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Reply to reviewer 1

The authors did a good job in addressing my reviewer comments and I can recommend publication of the manuscript. Here are a few minor points where communication remains unclear in my opinion:

- 5 l. 462: "The main consequence of this simplification is that the diffusion of a compound is calculated as if the compound has the same affinity with every layers." - This is unclear, what is meant with "affinity" here?

Our reply: affinity refers to the activity between the compound, which diffusion is calculated, and the compounds of the particle phase. The sentence is replaced by "The main consequence of this simplification is that the diffusion of a compound is computed assuming identical affinity across all layers, where this affinity represents the compound's activity relative to the other particle-phase constituents."

10 l. 609: "reaction rate multiplied by pH" - Do you mean this literally, as in a simple product? Is the reaction rate so directly correlated with pH?

Our reply: "reaction rate multiplied by pH" is replaced by "reaction rate multiplied by the activity of H⁺ ion"

15 *Figure 10: Is there also exchange between the intermediate layers and the interface layer? I cannot see an arrow between them.*

Our reply: One of the arrows was placed between the core layer and the interface layers instead of being placed between the intermediate layers and the interface. As the implicit method of Couvidat and Sartelet (2015) does not represent explicitly diffusion, The process is represented by a exchange fluxes between the interface layer and inner layers (that are represented by the double-headed arrows at the bottom of the figure).

20 The new version of the figure:

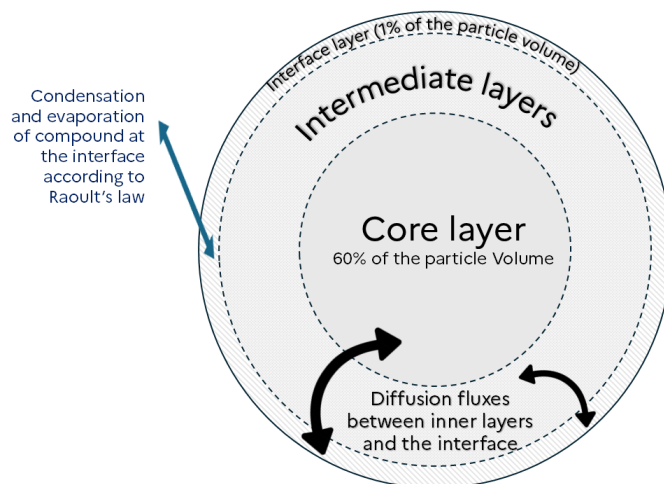


Figure 1. Illustration of implicit treatment of diffusion inside particle.

Reply to reviewer 2

1. The following question has not been addressed: While discussing results (e.g. L 303-306, Figure 8 etc.), the authors states what the results shows, but don't discuss why that's happening. The readers will appreciate if they get to know for e.g., why SOA yields are increasing/decreasing in the presence of NO_x.

25 **Our reply:** The following sentence is added line 331: "Differences in the simulated concentrations and their temporal evolution among the implicit, quasi-explicit and GENOA-reduced schemes arise from the richer formation pathways included in the quasi-explicit and GENOA-reduced mechanisms." The following sentence is added line 346: "The higher concentrations may be attributed to RO₂-HO₂ reaction rates, which tend to yield more highly oxidized monoterpene degradation products."

2. Although I appreciate the use of $\mu\text{g m}^{-3}$ for gas phase concentrations, it would intuitively make sense to address the gas-phase concentrations of species in ppm or ppb.

30 **Our reply:** We deliberately use $\mu\text{g m}^{-3}$ for all species, including gas-phase compounds, in order to maintain consistency across particulate and gaseous pollutants. Expressing concentrations in mass units is standard practice in atmospheric chemistry and air-quality modelling. It avoids ambiguities related to temperature and pressure assumptions inherent to volume-based units (ppm or ppb), ensuring internal consistency across the modelling framework. For these reasons, we retain $\mu\text{g m}^{-3}$ throughout
35 the manuscript. It is also the main concentration unit used within the code.

3. L296-298: Referring to Fig 4: these differences are barely visible in the plot. Perhaps the authors will think about providing percentage increase or decrease w.r.t the reference to indicate the difference. Our reply: The sentence "They are also lower than the reference with higher NO₂ levels in the first 1.5 hours of the simulation but higher after that, in opposition to the simulation
40 with the near-explicit scheme." corresponds to small variations that are very meaningful and hence it has been removed. Why

was it removed if was meaningful?

Our reply: Yes, indeed, the differences are barely visible in the plot and we consider them not to be significant. We also note that in our previous reply, the word "not" was inadvertently omitted. The sentence "They are also lower than the reference with higher NO₂ levels in the first 1.5 hours of the simulation but higher after that, in opposition to the simulation with the near-explicit scheme" referred only to very small variations that are **not** meaningful from a scientific perspective. For clarity and to avoid over-interpretation, this sentence has therefore been removed from the revised manuscript.