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Interactive comment on "A single-column particle-resolved model for simulating the vertical distribution of aerosol mixing state: WRF-PartMC-MOSAIC-SCM v1.0" *by* Jeffrey H. Curtis et al.

Anonymous Referee #1

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General comments:

This paper presents a stochastic method to simulate in 1D the vertical turbulent diffusion and dry deposition of particles in the atmosphere. The dynamic of aerosols is resolved using the previously developed PartMC-MOSAIC model, which computes stochastically the dynamic evolution of aerosols, taking into account their mixing states. The paper is well written. The approach is interesting to model aerosol concentrations in the atmosphere without assumption on their mixing state. However, the paper needs some clarification before publication. I recommend publication after the specific com-

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ments below are addressed.

Specific comments:

- Why do we need to simulate stochastically the vertical transport of particles? Gas/phase condensation/evaporation if done in a deterministic way, so why not vertical transport?

- The explicit vertical transport numerical scheme presented here may be quite expensive in terms of CPU cost for further 3D applications. Could the stochastic method be applied to implicit or semi-implicit scheme for solving vertical diffusion? Could it be less CPU expensive to use an implicit or semi-implicit scheme without a stochastic method?

- p2, l19-21: No, 3D chemical transport models that resolve additional mixing state information are not all focused on black carbon, see Zhu et al. 2016A, 2016b. To lower the computational cost of resolving the mixing state, they considered the mixing state of groups of chemical compounds, with 3D applications over Greater Paris.

Zhu S., Sartelet K., Zhang Y., Nenes A., Three-dimensional modelling of the mixing state of particles over Greater Paris J. Geophys. Res. Atmos., 121, doi:10.1002/2015JD024241, 2016a.

Zhu S., Sartelet K., Healy R., Wenger J., Simulation of particle diversity and mixing state over Greater Paris: A model-measurement inter-comparison. Faraday Discussions, 189, 547 - 566, DOI: 10.1039/C5FD00175G, 2016b.

- p5, l5-10/ Wouldn't it be more realistic to set the upper boundary condition to some value (0 or values given by a larger-scale model)? Emissions could also be taken into account at the surface as lower boundary conditions.

- p6 l5: have you tried to simulate transport before PartC and MOSAIC rather than after?

- p6 l28: How is determined the computational volume Vk from the grid cell? Please

add a short description here.

- p12. The details of the calculation are hard to follow. You should consider putting it in Appendix and adding more details, and only keep equations (37) to (39) in the paper. Equations (40), (41) could be put in place of equation (26), and the equations used for sampling can be presented with a with the whole explanation in Appendix. In the main part of the paper, you could just keep the explanation of what equations 40 and 41 have to be rewritten (because they are not independent as I understand). I assume that equation 31 is true because max() min() = 1. So it would add clarity to the paper to have more details in the Appendix about the equations through the calculation (min()pG = min(1/gamma,1) etc).

- p13. L13. What are the unsampled particles? Are they linked to Vk? Do they appear because the maximum transport term is considered rather than gain and loss? Why did they not appear in equation 25 of p10?

- p14. Using the algorithm presented here, how are we sure that in a time step the particles are not transported to levels k-2 or k+2?

- p15, p16, p17. You should consider putting the detailed algorithm in Appendix.

- How are emissions treated? At what stage of the algorithm?

- p20, Figure 6. Does this mean that the number of computational particles needs to be 10ˆ6 for atmospheric applications?

- p22. L 17. If there is a source of emissions in the domain, is this criterion modified at the point of emissions?

- p29. L7-10. How are nitrate concentrations impacted by the aerosol mixing state?

Technical comments

- p7, figure 1: z k+1 2 should probably be replaced by z k+1/2 and z k-1 2 should probably be replaced by z k-1/2

- p26, Figure 11. Use the same scale, at least for BC, SO4 and SOA.

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