Atmos. Chem. Phys. Discuss.,
doi:10.5194/acp-2016-1052-RC1, 2017
© Author(s) 2017. CC-BY 3.0 License.

Atmospheric Chemistry and Physics
Discussions
Open Access
EGU

Interactive comment on "An efficient approach for treating composition-dependent diffusion within organic particles" *by* Simon O'Meara et al.

Anonymous Referee #2

Received and published: 8 February 2017

The manuscript by O'Meara et al. describes a scheme that can efficiently treat the composition-dependent diffusion problem within aerosol particles. They used an improved numerical model as a benchmark, and developed a set of parameterizations for the correction of analytical solutions. This scheme was further implemented in the model MOSIAC to simulate the evolution of particle number size distribution. I think this is a timely paper as the non-liquid state and the associated slow in-particle diffusion has become a hot topic in current atmospheric chemistry research. This study was conducted carefully and the paper is informative. I would recommend publication in ACP once the authors address the specific comments below.

Specific comments

1. The authors mentioned water as an important plasticizer for organic particles. I think

this is also one of the motivations to develop such a composition-dependent diffusion model. However, it appears that the proposed correction scheme cannot be directly applied to the water/organic aerosol system as the molar volume ratio is far from the 1:1 ratio assumed in the simulations. This caveat should be discussed more explicitly in the manuscript.

2. It is not clear how the in-particle diffusion of the non-volatile component was considered in the model. It seems that Eq. 1 can be applied to both the semi-volatile and non-volatile components. If that is the case, does the value of D in Eq. 2 represent both D_sv and D_nv? This assumption is reasonable for the semi-volatile/non-volatile system discussed in this paper. These diffusivities, however, need to be treated separately if molecular sizes are vastly different (such as water/organics). Some more discussions would be helpful.

3. Page 2 Line 13: "Unlike gas-phase diffusion, which is already accounted for in regional-scale models by equations of gas/particle partitioning...". Equations of gas/particle partitioning not always account for gas-phase diffusion. Many models treat the gas/particle partitioning as equilibrium partitioning, i.e., gas-phase diffusion was not explicitly considered. However, it might be true that the timescale of gas phase diffusion is short enough compared to the typical time step in atmospheric models. Some models may use a dynamic gas/particle partitioning scheme where gas-particle mass transfer rates are taken into account. Please revise this sentence to be more specific.

4. Page 6 Line 3: The meaning of "ve Δxs,sv" is not clear. What does "ve" stand for? Some descriptions for "+ve Δxs,sv" and "-ve Δxs,sv" might be needed in the caption of figure 1, too (condensation and evaporation?).

5. Figure 3: It appears that the value of correction factor can be large even there is no composition dependence of D (pink and green lines in Fig. 3). This inaccuracy due to changing particle size could be further emphasized in the discussions and conclusions, too.

CC BY

6. Figure 9a: instead of showing the discrepancy between the models with/without the correction, I think it would be better to show the difference for each model with respect to the numerical solution. This may help the readers to understand how the results of composition-dependent model are improved compared with the model with a constant D.

Technical comments:

Page 5 Line 14: "by a factor or e"->"by a factor of e"

Interactive comment on Atmos. Chem. Phys. Discuss., doi:10.5194/acp-2016-1052, 2017.