

Interactive comment on “Mass Accommodation and Gas-Particle Partitioning in Secondary Organic Aerosols: Dependence on Diffusivity, Volatility, Particle-phase Reactions, and Penetration Depth” by Manabu Shiraiwa and Ulrich Pöschl

Anonymous Referee #3

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To date, Fuchs-Sutugin (F-S) approximation of mass-transport kinetics at the gas-particle interface with a fixed mass accommodation coefficient has been commonly in many models. In this work, the authors introduced an effective mass accommodation coefficient which considers penetration depth, surface accommodation coefficient, volatility, bulk diffusivity, and particle-phase reaction rate constant. They also suggest that this new coefficient and its dependence on these various parameters should be considered in the future when the F-S approximation is used to simulate gas-particle

interactions, in particular for viscous or semi-solid organic aerosols, which are commonly found in the atmosphere. The paper is well written and concise. It also provide new method for simulating SOA formation and evaluation. I support the publication of this work in ACP and have some minor comments below.

Comments

Line 194, “We simulate the temporal evolution of partitioning and equilibration of semi-volatile organic compounds (SVOC) with $C_0 = 100 \mu\text{g m}^{-3}$ and $D_g = 0.1 \text{ cm}^2 \text{ s}^{-1}$ interacting with non-volatile seed particles with a number concentration of 5000 cm^{-3} , an initial diameter of 200 nm, and a surface accommodation coefficient as $a(0) = 1$. For the SVOC, we assume initial gas- and particle-phase concentrations of $2 \mu\text{g m}^{-3}$ and $0 \mu\text{g m}^{-3}$, respectively. The particles are assumed to be either liquid with a bulk diffusion coefficient $D_b = 10^{-7} \text{ cm}^2 \text{ s}^{-1}$ or semisolid with $D_b = 10^{-15} \text{ cm}^2 \text{ s}^{-1}$.” Can the authors elaborate and justify why these parameters are chosen for their simulations? A typical condition for ambient conditions or laboratory studies?

Line 214, “For liquid particles with fast surface-bulk exchange and bulk diffusion ($D_b = 10^{-7} \text{ cm}^2 \text{ s}^{-1}$), $a(x)$ remains close to $a_s = a(0) = 1$, and all models yield the same result of fast mass transfer from the gas to particle phase and equilibration within one second.” Have the authors shown these results in the manuscript?

Line 235, “At long timescales ($> 1 \text{ h}$), the partitioning is reasonable well captured by both the MOSAIC approximation using a two-film approach of bulk diffusion (Zaveri et al., 2014) as well as the simple F-S approximation accounting for the influence of penetration depth with the effective mass accommodation coefficient, a_{eff} , newly introduced this study.” Can the authors comment how the simple F-S approximation accounting for the influence of penetration depth with the effective mass accommodation coefficient can be improved or used at short timescales ($< 1 \text{ min}$)?

Line 253, “Model results for SVOC partitioning plus reactive uptake with different rate coefficients in semisolid aerosol particles are shown in Figure 2b.” Can the authors

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elaborate how to choose these first-order bulk reaction rate coefficients ($k_b = 0, 10^{-4}, 10^{-3}, 0.01, 0.1 \text{ s}^{-1}$)?

Line 263, “Figures 3a and 3b show how the effective mass accommodation coefficient a_{eff} depends on volatility and bulk diffusivity as related to particle phase state and viscosity according to the Stokes-Einstein relation (Shiraiwa et al., 2011).” What are the timescale used in these simulations (e.g. $< 1 \text{ min}$, $1 \text{ min to } 1 \text{ hr}$ or $> 1 \text{ hr}$)? Would the simulated results affect by the timescale selected for the simulations (e.g. $< 1 \text{ min}$ vs. $> 1 \text{ hr}$)?

Line 263, For Figure 4, what are the timescale used in these simulations (e.g. $< 1 \text{ min}$, $1 \text{ min to } 1 \text{ hr}$ or $> 1 \text{ hr}$)? Would the simulated results affect by the timescale chosen for the simulations (e.g. $< 1 \text{ min}$ vs. $> 1 \text{ hr}$)?

Summary and conclusions. In this section, can the authors discuss how an effective mass accommodation coefficient can be extended to apply for aerosols containing both inorganic and organic species? How the phase separation and morphology can be accounted in the effective mass accommodation coefficient?

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