

Interactive comment on “Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions: Part 1 – general equations, parameters, and terminology” by U. Pöschl et al.

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1. The manuscript presents the model of the heterogeneous reactions of two species, X and Y, which can adsorb on the liquid aerosols. The model was built in the suggestion that the molecules Y form a surface layer and molecules X can react with molecules Y. The analytical expressions of the reactive uptake coefficient for the gas phase species X were derived on the base of the Langmuir-Hinshelwood mechanism under steady-state conditions due to the interface reactions with Y. This model postulated that in the

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calculation of the surface concentration of the species X (coverage) the mass-transport from the interface to the bulk may be ignored, see Eq. (84), Eq. (33-34), (38-40). Also, molecular dynamics simulations demonstrated that there is no large activation barrier between the gas phase and liquid-vapor interface to the insertion of an organic molecule into the interface [C. Girardet and C. Toubin, Surface Science Reports 44 (2001) 163.]. However, there is a small energy barrier (~ 1.5 kcal/mol) between the liquid-vapor interface and the bulk liquid [R. S. Taylor, D. Ray and B. C. Garrett, Journal of Physical Chemistry B 101 (1997) 5473].

2. For atmospheric modeling, the uptake process is usually considered on spherical aerosols. In this case, the contribution of the geometry factor may be considerable. The function of the size dependence was taken into account in the Eq. (68). This equation suggests that the boundary conditions formulated by Hanson [J. Phys. Chem. B, 1997, 101, 4998-5001] are the same for the model developed by Poschl et al. This suggestion requires additional confirmation because of the obvious strong dependence of surface concentration on the bulk concentration X .

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