

# Gas phase diffusion coefficients of atmospheric reactive trace gases and Knudsen numbers for gas uptake calculations

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The interactions of reactive trace gases with atmospheric particles (i.e. multiphase reactions) play important roles in many aspects of atmospheric chemistry (Kolb et al., 2010). Diffusion of gas molecules to the surface is the first step for all gas-surface reactions, and it can influence and sometimes even limit the overall rates of these reactions (Pöschl et al., 2007). So far, however, a database of gas phase diffusion coefficients for reactive trace gases of atmospheric interest is not available.

We (Tang et al., 2014; Tang et al., 2015) have compiled and evaluated, for the first time, the diffusivities (pressure-independent diffusion coefficients) of atmospheric reactive trace gases reported in the literature. The measured diffusivities are also compared with estimated values using Fuller's semi empirical method. It is found that the differences between the measured and estimated diffusivities is typically <30% for inorganic compounds and <10% for organic compounds, and therefore Fuller's method can be used to estimate the diffusivities of trace gases if experimental data are not available.

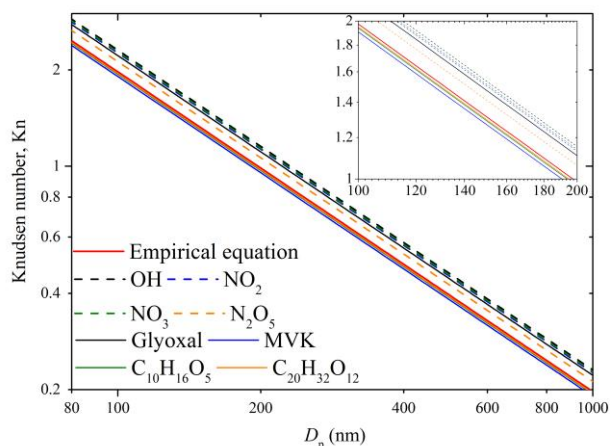


Figure 1. Knudsen numbers (Kn) for the uptake of four organic compounds (glyoxal, MVK, C<sub>10</sub>H<sub>16</sub>O<sub>5</sub>, C<sub>20</sub>H<sub>32</sub>O<sub>12</sub>) and four inorganic compounds (OH, NO<sub>2</sub>, NO<sub>3</sub>, and N<sub>2</sub>O<sub>5</sub>) onto aerosol particles as a function of particle diameter in 760 Torr air. Knudsen numbers calculated using the empirical equation (Eq. 11) we propose in this work are also plotted.

We further found that as shown in Figure 1, different gas molecules, including both organic and inorganic compounds, exhibit similar Knudsen numbers, although their gas phase diffusivities may vary over a wide range. We proposed a simple equation to calculate

Knudsen numbers, only as a function of particle diameter and pressure:

$$Kn = \frac{2}{d_p} \cdot \frac{\lambda_p}{P} \quad (E1)$$

where  $d_p$  is the diameter of the spherical particle (cm) and  $P$  is pressure of air in atm. The pressure-normalised mean free path,  $\lambda_p$ , which is equal to 100 nm atm, is a near constant generic parameter we introduce. This simplification has the potential to reduce the computational expense, especially for regional and global models with process based gas particle interactions.

A kinetic multi-layer model of gas-particle interaction (Shiraiwa et al., 2012) was used to illustrate the effects of gas phase diffusion on the condensation of organic compounds with different volatilities. The results show that gas-phase diffusion can play a major role in determining the growth of secondary organic aerosol particles by condensation of low-volatility organic vapours.

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