Mass Accomodation Coefficient for Nanoscale Aerosol Particles

Levdansky, Valerij Vladimirovič
2012

MASS ACCOMMODATION COEFFICIENT FOR NANOSCALE AEROSOL PARTICLES

Valeri LEVDANSKY[1,2], Jiří SMOLÍK[2], Vladimír ŽDÍMAL[2], Pavel MORAVEC[2]

[1]Heat and Mass Transfer Institute NASB, Minsk, Belarus
[2]Institute of Chemical Process Fundamentals AS CR, v.v.i., Prague, Czech Republic

Keywords: nanoparticles, size effect, mass accommodation coefficient

INTRODUCTION

The influence of size effects on physicochemical transformations and transfer processes in the heterogeneous systems with nanoobjects attracts increasing attention of researchers. These problems are of interest for nanotechnology and atmospheric physics. Size effects can influence the cohesive energy as well as the activation energies of vacancy formation and diffusion of atoms in the nanoscale particles (Vanithakumari and Nanda, 2008). Phase transitions (including nucleation) in aerosol systems with nanoscale particles (clusters) also depend on the nanoparticle size (Levdansky et al., 2010). Hear we discuss the size dependence of the mass accommodation coefficient γ in the gas–nanoparticle system.

RESULTS AND DISCUSSION

The value of γ depends on the rate constants for adsorption (k_{ads}), desorption (k_{des}) and absorption (k_{abs}) of gas molecules. Taking into account the relation between the sticking coefficient α_s and the value of k_{ads} ($\alpha_s = 4k_{ads}/v$, where v is the mean thermal velocity of gas molecules) and the equation for the mass accommodation coefficient (Crowley et al., 2010), the value of γ can be written as

$$\gamma = \frac{4k_{ads}k_{abs}}{v(k_{abs}+k_{des})}. \tag{1}$$

In view of the size dependence of k_{ads}, k_{des} (Murzin, 2009) and k_{abs} (Levdansky et al., 2009) in the case of nanoscale particles we can write following equations for mentioned rate constants:

$$k_{ads} = k_{ads,\infty} \exp\left(-\frac{4\alpha_{ads}\sigma V_m}{dRT}\right), \tag{2}$$

$$k_{des} = k_{des,\infty} \exp\left(\frac{4(1-\alpha_{ads})\sigma V_m}{dRT}\right), \tag{3}$$

$$k_{abs} = k_{abs,\infty} \exp\left\{\frac{Q_{abs,\infty}}{RT}\left[1-\exp\left(-\frac{4\delta}{\delta+d}\right)\right]\right\}, \tag{4}$$

where d is the particle diameter, $k_{ads,\infty}$, $k_{des,\infty}$, $k_{abs,\infty}$ are respectively the rate constants for adsorption, desorption and absorption for bulk matter, σ is surface tension for the nanoparticle (it is assumed for simplicity to be size-independent), α_{ads} is the Polanyi parameter for the adsorption rate constant, V_m is the molar volume of the substance forming the condensed phase, R is the gas constant, T is the temperature, δ is the Tolman length, $Q_{abs,\infty}$ is the activation energy for transition of molecules from the adsorption to absorption state for bulk matter.

First, let us consider the limiting case when $k_{des} >> k_{abs}$ and $d >> \delta$. Under the above-mentioned assumptions, the following equation for the value of γ can be written:

$$\gamma = \gamma_1 = \gamma_{1\infty} \exp\left[\frac{4Q_{abs,\infty}}{RTd^*}\left(1 - \frac{\sigma V_m}{Q_{abs,\infty}\delta}\right)\right], \tag{5}$$

where $\gamma_{1\infty} = 4k_{ads,\infty}k_{abs,\infty}/(vk_{des,\infty})$, $d^* = d/\delta$.
It is seen that in the case of the positive exponent in Eq. 5 the value of γ increases with a decrease in d^*. In the case when $k_{des} << k_{abs}$ and $d >> \delta$ the value of γ can be presented as

$$\gamma = \gamma_2 = \gamma_{2\infty} \exp\left(-\frac{4\alpha_{ads}\sigma V_m}{RTd^*\delta}\right), \tag{6}$$

where $\gamma_{2\infty} = 4k_{ads,\infty}/v$.
It is seen from Eq. (6) that in the considered case the value of γ decreases with a reduction in d^*. It is worth noting that the size dependence of surface tension can also affect the value of γ.

CONCLUSIONS

Thus, it is shown that the size dependence of the rate constants for adsorption, desorption and absorption of gas molecules in the gas–nanoparticle system can affect the mass accommodation coefficient. The value of the mass accommodation coefficient depending on the system parameters can both increase and decrease with a reduction in the nanoparticle size.

ACKNOWLEDGEMENTS

This work was supported by GAAVCR project IAA200760905 and GACR project 101/09/1633.

REFERENCES

Crowley J.N., Ammann M., Cox R.A., Hynes R.G., Jenkin M.E., Mellouki A., Rossi M.J., Troe J., Wallington T.J., Evaluated kinetic and photochemical data for atmospheric chemistry: Volume V – heterogeneous reactions on solid substrates, *Atmos. Chem. Phys.*, 10, 9059–9223 (2010).

Levdansky V.V., Smolik J., Moravec P., Impurity trapping by aerosol particles, *Aerosol Air Qual. Res.*, 9, 257–265 (2009).

Levdansky V.V., Smolik J., Moravec P., Size effects in physicochemical transformations in aerosol systems with nanoparticles, *Int. Commun. Heat Mass Transfer*, 37, 593–595 (2010).

Murzin D.Yu., Thermodynamic analysis of nanoparticle size effect on catalytic kinetics, *Chem. Eng. Sci.*, 64, 1046–1052 (2009).

Vanithakumari S.C., Nanda K.K., A universal relation for the cohesive energy of nanoparticles, *Phys. Lett. A*, 372, 6930–6934 (2008).