Atmos. Chem. Phys. Discuss., 15, C1469–C1471, 2015
www.atmos-chem-phys-discuss.net/15/C1469/2015/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Compilation and evaluation of gas-phase diffusion coefficients of reactive trace gases in the atmosphere: volume 2. Organic compounds and Knudsen numbers for gas uptake calculations" *by* M. J. Tang et al.

Anonymous Referee #3

Received and published: 9 April 2015

This manuscript presents compares gas phase diffusivities inferred from experiments (compilation of values reported in the literature) with gas phase diffusivities calculated using the method by Fuller et al. Based on the experimental values, preferred values are given and uncertainties are obtained by comparison within experimental data and with the calculated values.

The authors use a kinetic multi-layer model (presented elsewhere) to give an example of gas phase diffusion on condensation of two different organic molecules chosen

because of their atmospheric relevance and different volatility.

I find the topic and presented results very interesting. I recommend that the manuscript is published after some revisions. I find that the manuscript could be improved in terms of notation and explanations. In addition I find that the section where the multilayer model is used should be improved. My concerns and suggestions are outlined below and I hope the authors will find them useful in improving their manuscript.

Major

I think something is missing in Equation (3b) – otherwise in the examples in Section 6 Cg,diff would be ~0.5 in all cases? Should it be 1/(1+gamma/Taudiff)?

The notation and the use of units is not quite consistent. In equation 1 the concentration of X in the gas phase is denoted [X]g and the unit is molecule cm-3. In Figure 3 gas phase concentration of compound I is denoted Cg,VOC and is presented in mass concentration units.

I suggest to include an equation similar to equation 1 but with mass units to make it easier for the reader to go from one notation and set of units to another.

It should be explained how [SS] can be calculated, or at least some references to where this is explained should be given.

Page 5465 line 19: the effective uptake coefficient is introduced. I assume this value is replacing gamma in Equation 1 ?, but this should be stated explicitly.

Equation (4): I suggest to explicitly write Tau_diff (dp) to emphasize that the gas transport coefficient depends on particle size.

The example using the multilayer model: In general this is a very short section, but very interesting. To me it seems a bit as an “add-on” as it is now. I think this section could be better explained and several parameters should be varied (e.g. particle size, initial concentration of VOC). Estimation of volatilities of low-volatile organic molecules

ACPD
15, C1469–C1471, 2015

is highly uncertain, this should be acknowledged in the text.

How is the “near surface gas phase” defined?

In the example the authors have chosen a particle diameter of 300 nm. According to figure 2 this gives a Knudsen number of $\sim$0.6 and using Equation 4 this corresponds to a gas transport coefficient of 1. Is this a special choice? If so, the reader should be made aware of this. Also – as mentioned above it would be relevant to make similar model runs varying one key parameter at a time and discuss the effects.

In the conclusion it says “We further find that all the compounds have very similar Knudsen numbers” – If I understand correctly this was not done for all compounds but only four organics?

Minor:

Page 5472: “The differences between the measured and estimated diffusivities are typically <10%” – should it not say: The differences between the preferred and estimated diffusivities are typically <10% ?

Figure 3 caption: I think red and black has been exchanged in the explanation of figures 3.b and d.

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 5461, 2015.