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Atmospheric Chemistry and Physics Discussions

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Interactive Comment

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 #2

Received and published: 3 April 2015

The manuscript compiles and discusses diffusion coefficients for organic trace gases, important in atmospheric chemistry. The compiled experimental data are compared to an estimation method by Fuller (in Reid et al. 1987). Based on both, preferred values are suggested. Details of the assessment are documented in IUPAC style in an extensive supplement. This all is excellent work and should be published in ACP. (I did not check the supplement for errors and typos.)

The authors may to consider two suggestions before final publication:

The first regards the representation of the deviation between preferred (experimental) values and the Fuller estimation. In my opinion deviation between preferred and estimated values point to a systematic problem, not to a statistical one. In this case I suggest to give the deviation with the suited sign (to indicate if Fuller over- or underestimate D), and not with +/-.

The second point regards the notation “Knudsen number of molecules”. I think this is misleading. The Knudsen number is a scaling factor for a certain problem and relates a particle radius to a free mean path e.g. of a condensing vapor. Kn determines dynamic regime of uptake for a given particle size. Kn “tests” if diffusion to a large particle (quasi motionless) or molecular kinetics rules by rationing the free mean free path (lambda) of the vapor to particle diameter. What the authors find invariant is lambda of the molecules. If I pluck in some numbers in Eq. 12 and consider the definition of Kn as lambda / Rp (Particle radius) then at 760 torr the lambda for many molecules including small inorganic is about 100nm, a typical value.

Therefore de facto mean free path is invariant not the Knudsen number. Of course I am convinced the authors know all this, but I am warning because the semantics is misleading, although in praxis this has no effect.

Minor comments:

page 5471, line 1-2: I suggest to mention one more time that “estimated refers to Fullers method. Something like: “. . .the difference between preferred and diffusivity estimated by Fuller’s method, then. . .”

page 5471, line 8: it would be helpful to give the value estimated by Fuller here for better comparison.

page5473, line 1: Is the estimated diffusivity for larger carboxylic acids larger or smaller than the "measured". Could internal hydrogen bonding lead to "unusal" molecular morphologies/folding or similar?

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page 5474, line 9: I suggest to state that the mean free path, which is approximated by Dp(X)/c(X), is relatively invariant and as a consequence Kn is similar for many vapors for a given particle size.

Typos

page 5467, line 14: use plural, “inorganic compounds” page 5471, line 8: singular, diffusivity page 5474, line 11: square

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