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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 #1**

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In this manuscript, the authors developed a database of diffusion coefficients for atmospheric trace gases. The goal is to use these diffusion coefficients to calculate the rate of gas uptake onto particles. The authors compiled an extensive list of coefficients and made recommendations, and also cited Fuller's method to estimate diffusivities. These diffusion coefficients are then applied to calculate Knudsen numbers and condensation into particles. The paper is clearly written, and the topic is relevant to the scope of Atmospheric Chemistry and Physics. This manuscript should be published after considering these comments:

- In general, the range in diffusion coefficients is small. It ranges from 30 to around 100 torr cm2 s-1, within 1 order of magnitude of each other. It seems to be that the difference between MVK and C20H32O12 is a result of its volatility, not diffusion coefficient. Why is it then an important task to compile gas-phase diffusion coefficients to correctly model condensation flux? It would seem to be that understanding volatility (which has an error of ∼2 orders of magnitude) is more important, and we can assume an average gas phase diffusivity of ∼0.1 cm2 s-1. Perhaps the authors can choose a better example?

- If gas phase diffusion becomes the limiting step for these ELVOCs to condense, can the authors comment on the relative importance of heterogeneous reactions of smaller molecules that lead to SOA formation (e.g. glyoxal dissolution and subsequent reactions) and larger molecules such as ELVOCs condensing onto particles? It would seem to me that heterogeneous reactions of smaller, more diffusive compounds can potentially be very important.

- In general, it would be nice to perform some sensitivity analysis. For example, the uncertainty in measurements could be used to investigate errors in the condensational flux. Also, the uncertainty in using Fuller's estimation (<10%) can also be investigated. My guess is that these uncertainties are quite small and have little overall effect on estimated condensational flux.

- Tables 1 and 2 list diffusivities of common gases. It would be useful to tabulate estimated diffusivities of common oxidation products, such as glyoxal, pinonic acid, IEPOX, which would be helpful for the SOA community. Fig. 2 lists some common oxidation products, but it would be nice to see the diffusion coefficients that went into the calculations listed in a table.

Minor comments: - I suggest rearranging Tables 1 and 2 so that the compounds are listed in increasing molecular weights or carbon numbers from top to bottom, not left to right.

- Pg. 5475 Equation (12): Particle diameter is usually in nm or um, so it may be more convenient to adjust the units in Dnorm (e.g. 150 torr um)
- Pg. 5464 line 24: “condendation” should be “condensation”
- Pg. 5467 line 13: insert “in” into “. . .used our previous work. . .”
- Pg. 5469 line 9: “differenciate” should be “differentiate”
- Pg. 5472 line 8: “multifuntional" should be “multifunctional”
- Pg. 5472 line 12: “tropshere” should be “troposphere”
- Pg. 5473 line 13: “tempereatures” should be “temperatures”
- Pg. 5474 line 11: “sqaure" should be “square”
- Pg. 5476 line 4: “assumed to consists” should be “assumed to consist”
- Pg. 5477 line 5: “alcoholes” should be “alcohols”
- Pg. 5486 Table 2 caption: “multifuntional" should be “multifunctional”
- Pg. 5488 Table A1 caption: “fours” should be “four”
- Pg. 5492 Figure 3: The units on the y-axis label are not shown correctly. I am guessing that they should be in ug m-3

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