

Interactive comment on “A new modeling tool for the diffusion of gases in ice or amorphous binary mixture in the polar stratosphere and the upper troposphere” by C. A. Varotsos and R. Zellner

Anonymous Referee #2

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The manuscript submitted by Varotsos and Zellner strives to define a general diffusive transport mechanism which operates in ice at cold temperatures. They do so by aggregating data from a few experimental efforts all of which are modeled as Arrhenius type behavior. Their primary argument is that the linear relationship between $\ln D_0$ and E (their notation), which for Arrhenius behavior is expected from examination of the governing equation, has a general form for heterogeneities in ice whose diffusion is governed by a vacancy mechanism. The authors argue that because of the generality of this mechanism this relation may be able to be used in order to derive diffusion coefficients for other impurity species in ice. The key to this argument is that for water ice it appears that diffusion of various species through the matrix is chiefly controlled

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by properties of the ice and not the diffusing species.

Although a careful reading of this paper has shown it to be sound, I cannot recommend it for immediate publication in its current form. I feel that short-comings do exist, which if addressed by the authors would greatly improve the quality and utility of the manuscript. Because the theoretical framework presented here is fairly straight forward, an important contribution of this paper is that it presents a review of existing experimental data. However, here it falls short of being comprehensive. For example more recent experimental evidence [1,2] is available for HCl and also includes results for heavy isotope diffusion in ice. I do not have comprehensive knowledge of the diffusion of species in ice literature, however, the authors should perform an exhaustive search in order to include as many studies as possible in their analysis. This will improve the parameter range of theoretical comparison and ultimately, if their findings hold, be more convincing.

Returning to the current manuscript, I also suggest that both Fig. 1 and Fig. 2 include some indication of error. At a minimum the error for D , used in Fig. 1, should be given in Table 1. Inspection of the table also makes it clear that the large error estimates in E will make a range of slopes in Fig. 2 possible. The author's primarily conclude that this slope could be used predictively, as such it should be constrained – to give the reader a sense of the potential accuracy of such a method.

Finally, because the motivation of these investigations is largely geophysical, I encourage the authors to address the potential effects of polycrystallinity. This is true in the cited experimental measurements as well as in the discussion and conclusions. It is known that the character of ice samples (single- vs. poly- crystals, degree of crystallinity, and orientational homogeneity) may play a role in species mobility [3]. The author's tangentially address this with their brief discussion of the potentially amorphous mixture results. Simple, explicit descriptions of the other cited experimental measurements, and a discussion of the potential effects of highly polycrystalline samples would also benefit readers.

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In short, the Varotsos and Zellner manuscript has a strong foundation, but appears to have ignored studies which could augment their work. Outlined additions to the figures and discussion would also be beneficial to the readers. Until these shortcomings are addressed I cannot support publication of the author's manuscript.

TECHNICAL NOTES: In the manuscript I was able to retrieve, I noted a few small copy editing errors. 1. In line 10 detected is misspelled as defected, but could be struck altogether as it is redundant. 2. Line 27, than is misspelled as that.

References

- [1] H. Lu, S. A. McCartney, and V. Sadtchenko, "Fast thermal desorption spectroscopy study of h/d isotopic exchange reaction in polycrystalline ice near its melting point," *Journal of Chemical Physics*, vol. 127, p. 184701, 2007.
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- [3] A. W. Rempel and J. Wettlaufer, "Isotopic diffusion in polycrystalline ice," *Journal of Glaciology*, vol. 166, no. 49, 2003.

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