Interactive comment on “Gas transport in firn: multiple-tracer characterisation and model intercomparison for NEEM, Northern Greenland” by C. Buizert et al.

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The authors would like to thank the referee for his / her careful reading of the manuscript and for the thoughtful comments.

The referee identified an important error in the work:
RC: “First the error: P15989 Eq. 3: The RMSD term that defined is very close to Chi-squared- per-degree-of-freedom. The only difference is that, to be a true chi-squared variable, the divisor “N” should be adjusted for the number of free parameters in the fit to the diffusivity. Unless this is done, the conclusion that ‘RMSD<1 implies conservative error estimates’ is not strictly valid. Consider the limiting case of three data points that are fitted with a parabola. This will always yield RMSD = 0, regardless of whether the errors are tiny or enormous. Minimizing a correctly formulated Chi-squared figure of merit will give exactly the same optimized diffusivity as minimizing RMSD, but the values of Chi-squared can be interpreted quantitatively. Fixing this will also require reworking the discussion surrounding figure 4. I recognize that determining the appropriate number of free parameters may not be a simple task (and this may be why the authors chose RMSD as a metric), but the interpretation of RMSD as it stands is, at best, only qualitatively correct, and may be simply wrong.”

We agree that interpretation of the RMSD as defined by Eq 3 in an absolute sense is incorrect, and that our statement about conservative error estimates is not justified. We see the advantage of having a model performance metric that can be interpreted in an absolute sense -leading up to this work some of us considered using a Chi-squared test for the diffusivity optimization. However, we believe a Chi-squared per degree of freedom, as suggested by the referee, is not suitable for this study for the following reasons:

- The Chi-squared test statistic is of the form:
\[ \sum \frac{(d_i - m_i)^2}{d_i} \]
where \( d_i \) and \( m_i \) are the data and model values, respectively. The division by the signal amplitude gives an almost infinite weight to tracers that approach zero in the lock-in zone, such as SF\(_6\) and several halocarbons. Our definition of the RMSD includes normalization with respect to amplitude implicitly through the \( \sigma_i \).

- The number of degrees of freedom relates to linear analysis (reflecting for example the number of independent eigenvectors that can be generated out of a linear model), while the diffusivity optimization is a non-linear problem. Apart from the
difficulty in establishing the degrees of freedom, their number also differs between the models (each modeler was free to decide how to optimize the diffusivity).

The main purpose of defining the RMSD is to have an objective way to tune the models. In the diffusivity reconstruction only relative changes in RMSD are considered (i.e. for what model configuration is the RMSD minimized). The RMSD as defined by Eq. 3 is suitable for this purpose. Our absolute interpretation of the RMSD is incorrect, and in a revised manuscript we will remove the statement about conservative error estimates. We will furthermore add the caveat:

“Differences in RMSD give information on the performance of models, or model configurations, relative to each other; the RMSD as defined by Eq. (3) should not be interpreted in an absolute sense.”

The referee further lists a number of concerns, suggestions and editorial comments. All cases where we will simply follow the suggestions of the referee are omitted from the response below.

RC: “On page 15980, line 11-12 the authors state that uncertainties in the atmospheric reconstruction used to tune the diffusivity “are a large source of potential error”. This is an important point and is underemphasized in the paper. It is only section 2.7 that any mention is made, and one can only assess the relative importance of the 7 potential sources of error by a careful reading of the supplementary material. Perhaps a table of the various sources of error would be a good addition to Section 2.7.”

We will include a table where for all 10 tracers the relative contribution of the 7 sources of uncertainty is given, averaged over the firn column.

RC: “Page 15988 and following: I really don’t like the use of the term “dispersion” for the transport that is occurring through mechanisms other than molecular diffusion. In classical (and quantum) physics, dispersion indicates propagation in which different components of a substance move at different speeds (light waves in dispersive glass leading to chromatic aberration, etc.). This is exactly the opposite of what is going on in the deep firn. Here, we know the transport is not molecular diffusion precisely because the different species do move at the same speed. Eddy diffusion, bulk transport, or some other term is far preferable.”

The term ‘dispersion’ has indeed not been used previously in the firn air literature. Dispersion has a variety of meanings in physics, including the one referred to in the referee comment above. In fluid dynamics the term dispersion is used for the spread of a solute by non-uniform flow (i.e. deviations from plug flow). The classical example is the spread of a solute in Poiseuille flow through a circular tube, where the shear flow increases the effective diffusivity of the tracer (referred to as Taylor dispersion, see e.g. R. Aris: on the dispersion of a solute in a fluid flowing through a tube, Proc. R. Soc. Lond. A, 1956). The term is also used widely for modeling of pollutants in ground water and atmosphere (e.g. from smoke stacks). On a microscopic scale dispersion is a combination of advection and diffusion. The models cannot resolve the microscopic flow patterns; in our macroscopic transport description we parameterize the effect by including a dispersive term. Mathematically dispersion is described by Fick’s law.

“Eddy diffusion” (sometimes also referred to as eddy dispersion) strictly speaking refers to mass transfer due to eddy motion and turbulence, which is not the case in the deep firn. In our view the term ‘bulk transport’ refers primarily to advective transport which does not cause mixing; by dispersion we mean precisely the enhanced diffusivity that arises from non-uniformities in the bulk motion.

What we believe to be going on in the deep firn is enhanced mixing due to viscous flow (Poiseuille flow) in combination with non-uniformities in bulk motion due to pore
We feel that the term ‘dispersive mass transfer’ captures these processes best. We will replace the term ‘dispersion’ with ‘dispersive mass transfer’ to distinguish it from other dispersion processes in physics.

RC: “Section 3.2: How is the transition between the diffusive zone and the lock-in zone defined? Is it simply where the molecular diffusivity goes to zero? The location of this transition is essential for successful model tuning. Presumably the objective tuning processes that are used for the various models automatically find this transition, but this is not clear in the manuscript.”

In section 2.2 we define the lock-in depth as the depth were gravitational enrichment stops (63 m). This roughly coincides with the depth where the effective molecular diffusivity approaches zero (i.e. gets reduced by several orders of magnitude). The models have complete freedom to tune the tortuosity, so the depth where molecular diffusion ceases can potentially vary. We will clarify this in revision.

RC: “P15993 Line 7-8: I can see how the values in Table 1 lead to the “spread of around 30%” for the mean age and FWHM, but this statement doesn’t look true to me for the spectral width. Please clarify.”

The spread in the spectral width $\Delta$ is larger (around 60%) because in the definition:

$$\Delta^2 = \frac{1}{2} \int_0^\infty (t - \Gamma)^2 G(z, t) dt$$

the width around the mean age $\Gamma$ is included as the square, which gives more weight to the edges of the distribution. The FWHM does not consider the edges so much. We will include numbers for the model spread in table 2 for clarity.

Supplementary material

Again, in what follows we will not include a response in cases where we will simply follow the suggestions of the referee in revision.

RC: “Section 2.7.2: This statement is not clear to me: “Since the uncertainty estimates do not have a temporal resolution better than a few years, we believe this approach to be valid.” I simply can’t make sense of it. What are the authors trying to say.”

The temporal uncertainties in the reconstructed history are mapped onto a depth scale using a preliminary diffusivity tuning for the CIC firn air model. The mean ages produced by the model might therefore be off by a few years. However, the uncertainty record used as an input in the firn model does not have a temporal resolution better than a couple of years to begin with; therefore the small timing errors of the preliminary model are not very relevant. This will be clarified in the text.

RC: “Section 3.2: Open porosity is not necessarily zero below the depth at which firn air samples can no longer be extracted (see, for example, Aydin et al, ACP 2010).”

We will include the reference. We have no measurements of open porosity, and we’ll have to rely on parameterizations which all give a very abrupt pore closure.

RC: “Table 15: What is the difference between the two versions of Scenario II?”

See section 4.2.2 of the main text. We force both a sine and a cosine scenario to reconstruct the wave amplitude.
RC: “Section 2.4.3: Uncertainties in the reconstructed atmospheric histories seem somewhat arbitrarily determined. For example, in the case of CO$_2$, why choose half of the offset? Why 2sigma for the recent Law Dome record and 3sigma for the older Law Dome record? These choices may be good ones, but they are completely unjustified.”

Indeed not all of the numbers are justified in the text. First, we chose not to give extensive reasoning behind all numbers for reasons of brevity. Second, it is very difficult to assign accurate and objective estimates back in time. Some choices will necessarily be subjective. For this reason we compared histories compiled by different people to get a feeling for how objective the estimates are. But different reconstructions can never be fully independent, since ultimately they will be based on the same (limited) datasets that are available.

In the case CO$_2$, our reconstruction for the most recent times are based on both Alert and Summit stations. Since NEEM is in between, we take the average of these two stations. We assign an uncertainty of half the offset since we cannot exclude the possibility that CO$_2$ mixing ratios over NEEM are identical to those at either station, rather than their average. The errorbars for Law Dome give the analytical measurement uncertainty. Going further back in time there is additional uncertainty because of dating, ice core $\Delta$age and changes in the inter-hemispheric gradient. The choice of progressively larger error bars when going back in time represent this.

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