

Reply to reviewer 2:

We thank reviewer 2 for the detailed examination of the presented work. This allows us to clarify some issues potentially not emphasized enough within our discussion manuscript. Therefore we will use this opportunity to address major issues together with detailed answers to the key points mentioned by the reviewers. Reviewer comments are given in italic letters whereas our replies are given in normal letters.

Point (1):

The method assumes that the forward problem (converting surface temperature to $d15N$) is completely described by the firn model, and that all variations in $d15N$ can be linked 1-to-1 to past surface temperature. It is thus no surprise that they can reconstruct the original temperature very accurately, because they know the exact accumulation rates and physics of the forward model. Unfortunately, that is not at all true in the real world.

We are well aware of the fact that this assumption does not hold true. Due to uncertainties and simplifications in firn densification and gas diffusion physics, uncertainties in common firn models and measurement data our assumption is only an approximation of the real world as mentioned by the reviewer. Therefore, we will discuss several issues in this reply to reviewer 2. Nevertheless we used this assumption here to show the functionality of the automated fitting algorithm. Detailed uncertainty estimations for a “real world” scenario as demanded by the reviewer are behind the scope of this work and will follow for the reconstructions using measurement data ($\delta^{15}N$, $\delta^{40}Ar$, $\delta^{15}N_{excess}$) in next publications. Again, the aim of this work is to present the automated gas isotope fitting algorithm applied to synthetic Holocene $\delta^{15}N$ data and to study the uncertainties emerging from the algorithm itself. Furthermore the focal question in this study is: what is the minimum final mismatch in $\delta^{15}N$ for Holocene data we can reach and what does this mean for the final temperature mismatches. Studying and moreover answering these questions makes it mandatory to create well defined $\delta^{15}N$ targets and related temperature histories, as we did here. It is impossible to answer these questions without using synthetic data in a methodology study. The aim is to evaluate the accuracy and associated uncertainty of the inverse method itself to then later (in a future study) apply this method to a real $\delta^{15}N$ dataset, for which of course the original driving temperature history is unknown.

The $d15N$ is influenced by variations in convective zone thickness (the CZ is ignored here altogether), firn layering that influences the lock-in process, melt layers and wind crusts, etc. Real data (as opposed to the synthetic data used) further suffer from analytical noise in the laboratory. All these things will reduce the ability to reconstruct temperature from $d15N$. Furthermore, our understanding of firn densification is incomplete, with several physical models giving different results, microstructure effects not included in models, and hypothesized influences of dust softening. All these effects remain unaccounted for, which further reduces the ability to use $d15N$. The authors use identical firn physics in the forward and inverse models, which is an idealization that is untenable.

Regarding the convective zone (CZ): The presented fitting algorithm was used together with the two most frequently used firn models for temperature reconstructions based on stable isotopes of air, the Schwander et al. (1997) model which has no CZ build in (or better a constant CZ of 0 m) and with the Goujon firn model (Goujon et al., 2003) (which assumes constant convective zone over time, that can easily be set in the code). This difference between the two firn models only changes significantly the absolute temperature rather than the temperature anomalies as it was shown by other studies (e.g., Guillevic et al. (2013), fig. 3). In the presented work, we show the results using the model from Schwander et al. (1997), because the differences between the obtained solutions using the two models are negligible besides a constant temperature offset of about 2.3K. Also, noteworthy is that there is no firn model at the moment which uses a dynamically changing CZ. Indeed, this should be investigated but requires additional intense work. Additionally, the knowledge of the time evolution of CZ changes for the time periods of millennia to several hundreds of millennia (in frequency and magnitude) is too poor to estimate the influence of this quantity on the reconstruction.

In addition the algorithm is able to fit $\delta^{15}N$, $\delta^{40}Ar$ and $\delta^{15}N_{excess}$ data as mentioned in the paper (e.g. in the abstract at line 17). In fig.1 we show unpublished data to clarify that the algorithm is usable for $\delta^{15}N_{excess}$ besides $\delta^{15}N$ data. Here the $\delta^{15}N_{excess}$ data from Kobashi et al. (2008) was used as the fitting target using the same approach. We reach a final mismatch (2σ) of 3.7 permeg, which is below the analytic measurement uncertainty of 5.0 to 9.8 permeg of the measurement data. We hope that this is convincing enough to show the functionality of our algorithm also for this quantity. The automated inversion of different gas isotope quantities ($\delta^{15}N$, $\delta^{40}Ar$,

$\delta^{15}\text{N}_{\text{excess}}$) provides a unique opportunity to study the difference of the gained solutions for the different targets and to improve our knowledge about the uncertainties of gas isotope based temperature reconstructions using a single firm model. Because of the “perfect physics scenario” as mentioned above it is not necessary to show the synthetic $\delta^{40}\text{Ar}$ and $\delta^{15}\text{N}_{\text{excess}}$ fits here, because the gained solutions are the same. This will be different when using measurement data. Here differences between the temperature solutions gained from the single targets ($\delta^{15}\text{N}$, $\delta^{40}\text{Ar}$, $\delta^{15}\text{N}_{\text{excess}}$) will become obvious due to several sources of signal noise. These differences will allow to quantify the uncertainties associated with processes mentioned by the reviewer.

Next, the presented algorithm is not dependent on the firm model, which leads to the implication that the algorithm can be coupled to different firm models describing firm physics in different ways. An automated reconstruction algorithm avoiding manual manipulation and leading to reproducible solutions makes it possible for the first time, to study and learn from the differences between the solutions. Differences that then can be assigned to different firm models and their shortcomings, resulting in more robust uncertainty estimates as was possible before. Thus, the algorithm provides the possibility to test firm models by fitting different targets and as mentioned before to learn from the differences between the solutions obtained by matching single targets. This is exactly the reason the algorithm was developed for.

Several studies have shown that on the cm-scale there is much variation in parameters like $d^{15}\text{N}$ and CH_4 , reflecting a staggered trapping of gas bubbles within the firm-ice transition zone. See e.g. Etheridge et al. (1992), Rhodes et al. (2016), and Mitchell et al. (2015). This may be relevant as the sample size is typically smaller than the average layer thickness.

Also that point is not related to the scope this paper. Within the scope of paleoclimate reconstruction, the pertinent focus is more on how to extract signals from gas isotope data rather than how to represent potential sources of signal noise. Of course signal noise (such as firm heterogeneity) should be included in the uncertainty estimation, which is planned in a future study dealing with modelling (among others) real $\delta^{15}\text{N}$ data. However, we will try to account for this question here. We fully agree, for the reconstruction using measurement data, it is necessary to keep cm scale variability in mind. Our view on this point can be summarized as follows: During the analytical analyses of ice core air data it is common to measure replicates for given depths, from which the measurement uncertainties of the gas isotope data is calculated using pooled-standard-deviation (Hedges L. V., 1985). Often it is not possible to take real replicates (same depth) and instead the replicates are taken from nearby depths. So, the cm scale variability is to some degree already included in the measurement uncertainty, because each measurement point represents the average over a few centimetres of ice. This is especially the case for low accumulation sites or glacial ice samples for which the vertical length of a sample (e.g., 10-25 cm long for the glacial part of the NGRIP ice core, Kindler et al., 2014) covers the equivalent of 20-50 yrs of ice at approx. 35 kyr b2k. Increasing the depth resolution of the samples would increase our knowledge of cm scale variability, for e.g. identifying anomalous layers that could have been rapidly isolated from the surface due to a high density layer (e.g., Rosen et al. (2014)). As this variability is likely due to heterogeneity in the density profile, this may not help to better reconstruct a meaningful temperature history, rather to observe the source of signal noise. To sum up: The cm scale variability, in many cases, is already incorporated in the analytical noise obtained from gas isotope measurements, due to analytical techniques themselves. Assuming the measurement uncertainty as Gaussian distributed, it is very easy to incorporate this source of uncertainty in the inverse modelling approach. This will increase the uncertainty of the temperature according to Eq. (9) in our manuscript using the presented approach. The same equation can also be used for the calculation of the uncertainty in temperature related to measurement uncertainty in general.

To answer the pertinent question of how to better extract a meaningful temperature history from a noisy ice core record, an excellent – but costly – solution is of course to use multiple ice cores. The GISP2 ice core has actually the chance to have a “sister ice core” drilled only a few kilometres apart (the GRIP ice core) and combining $\delta^{15}\text{N}$ -based temperature reconstructed from both ice cores is likely one of the best ways to overcome potential cm scale variability. A comparison of ice cores that were drilled even closer might be even more advantageous.

Gas diffusion and trapping smooths out the $d15N$ signal, which provides a fundamental limit on the time resolution at which surface temperature is recorded and could potentially be reconstructed.

The duration of gas diffusion from the top of the diffusive column to the bottom where the air is closed off in bubbles is for Holocene conditions in Greenland approximately in the order of 10 yr (Schwander et al. 1997), whereas the data resolution of the synthetic targets was set to 20 yr to mimic the measurement data from Kobashi et al. (2008) with a mean data resolution of about 17 yr (see section 2.4: “Generating synthetic target data”). In the study of Kindler et al. (2014) it was shown that a Glacial Greenland lock-in depth leads to a damping of the $\delta^{15}N$ signal of about 30% for a 10 K temperature rise in 20 yr. We further assume that the smoothing according to the lock-in process is negligible for Greenland Holocene conditions according to the much smaller amplitude signals and shallower lock-in depth for Holocene conditions.

From the above it is clear to me that the precision that the authors state for their method is a meaningless number, that teaches us nothing about how well $d15N$ can reconstruct temperature. A more interesting approach would be to include these fundamental uncertainties in a stochastic way, and see how well the method works under realistic settings. The synthetic data could e.g. be generated with a different firn physics description, and should be subject to CZ fluctuations, LIZ thickness variations and analytical noise.

This is obviously a misunderstanding. Indeed we did not mention that the mismatch in $\delta^{15}N$ and the therefrom calculated temperature range would correspond to an uncertainty of temperature reconstructions. This range is only the uncertainty part that directly relates to the inversion model approach and does not include any other uncertainties that exist. In the “perfect world” scenario it should be theoretically possible to reach a final mismatch of zero for $\delta^{15}N$ as well as for temperature. The reason why this was not reached in our study is related to the memory effects in the ice sheet model which leads to a rising computational effort for reaching very low mismatches. An improvement of one section of the time series will be paid by degradation in another part. To circumvent the computational demand we developed the correction step (step 4, section 2.4.4), which accounted for this memory effects. This means that in finite time there has to be a limit the algorithm can reach, which is exactly characterized by the final mismatches presented here.

Additionally, in the perspective of making a complete uncertainty budget for a temperature history reconstructed based on $\delta^{15}N$ data (again, as will be done in a future publication), this uncertainty value for the inverse modelling method, being not zero, cannot be neglected and should therefore be taken into account.

Point (2):

There are 2 fundamental inputs into the model, namely temperature and accumulation rate. The authors assume the latter is known with zero uncertainty (both in values and age model). This is a very unrealistic assumption. Even if the layer-count were perfect (which it is not), correcting for ice thinning has a fundamental uncertainty. Especially in the early Holocene, this can easily exceed 10%. As the method fits the $d15N$ data, all accumulation errors are mapped into the temperature reconstruction. This is not accounted for...As an aside, the authors convert the accumulation record from Cuffey et al. onto the GICC05 scale, which makes it internally inconsistent because the accumulation rate is the derivative of the age scale, so changing the age scale should change the accumulation values. Since the method is sensitive to the decadal-scale accumulation variability, it may be insufficient to use this crude approach.

Answer for the point on the conversion of the Cuffey accumulation record to the GICC05 time scale: We think this comment arose from a lack of details given in the paper. Therefore we describe in the following in more detail the procedure we used to produce the finally used accumulation rate data for our modelling work. The original accumulation rate for the GISP2 ice core is the one published in Cuffey and Clow (1997), produced using an ice flow model adapted to the GISP2 location. The accumulation rate used to feed the ice flow model was optimised in order to match the time scale from Meese et al. (1994) for the Holocene, based on annual layer counting. Seierstad et al. (2014) transferred the GISP2 chronology to the GICC05 reference timeframe using multiple match points to the NGRIP and GRIP ice cores, both already on GICC05. We used these match points and modified the GISP2 duration in between match points linearly in order for the considered interval to match exactly the GICC05 duration. This way, the detailed GISP2 annual layer counting information is kept, but is only stretched/compressed in time. This was done for all intervals in between two match points. The accumulation

data were then re-calculated accordingly, as obviously (as stated by the reviewer) this is needed in order to keep the same total amount of ice accumulated at the GISP2 site. Actually, to obtain an even better consistency, the best would be to re-run the Cuffey and Clow ice sheet model, using the GICC05 timescale as target timescale, and use the resulting accumulation rate data (but this is beyond the scope of this study).

Furthermore, as we have shown in the paper in section 2.4 “Accumulation rate input”, the accumulation rate variability has a minor impact compared to the temperature on the variability of the $\delta^{15}\text{N}$ data in the Holocene (see also fig.A02). The influence of the quantities, accumulation rate or temperature, into the temperature reconstruction is not equal, the accumulation rate variability during the Holocene explains about 12 to 30% of the $\delta^{15}\text{N}$ variability. 30% corresponds to the 8.2 kyr event and 12% for the mean of the whole Holocene period including the 8.2 kyr event. Hence the influence of accumulation changes is generally below 10% during the Holocene. If the accumulation is assumed to be completely correct then the missing part will be assigned to temperature variations. Also in section 2.3.1 we show that the polynomial degree in temperature is more important than for the accumulation for the calculation of a polynomial transfer function (see line 3-6 at page 5 and fig.S02). Nevertheless for the fitting of the Holocene measurement data we will use all three accumulation rate scenarios as shown in fig.S01. The difference in the reconstructed temperature arising from the differences of these three scenarios will be used for the uncertainty calculation as well and is most likely higher than the uncertainty arising from the conversion of the accumulation rate data to the GICC05 timescale.

Point (3):

The authors have no way of validating that their Delta-age is correct, which is critical to constrain the timing of climate change. In all $d15\text{N}$ modeling studies I'm aware of, the use of $d18\text{O}$ as a temperature template ensures that Delta-age is correct. In particular during abrupt events, the timing of gas and ice signals gives you Delta-age. This information is lost in their method, which is completely independent of $d18\text{O}$. If the modeled Dage is off by 50 years (which is easy to do in Greenland, particularly during the glacial), the timing of the temperature solution is also off by 50 years. It would be interesting to run their algorithm on data from the last deglaciation, and see whether it reproduces the timing of abrupt change as seen in $d18\text{O}$. Because Deltaage is underconstrained, the timing of all reconstructed high-frequency temperature variations is uncertain.

We thank the reviewer for mentioning that point, since we have not explicitly discussed the behaviour of the Δage agreement in the paper and we will catch up on this. The Δage adjustment in the Holocene case is related to the smooth temperature solution calculated by the Monte Carlo part of the algorithm. If a smooth temperature solution is found which creates a robust long term signal in $\delta^{15}\text{N}$ the gas age - ice age difference from that model output is used to calculate the high frequency information and to find the right timing for adding the high frequency signal to the smooth temperature solution as it was explained in section 2.4.2 (page 9, lines 11-13) and section 2.4.3 (page 9, lines 18-23). As the measurement target data is set on the ice age scale (like all gas isotope data after measurement) and the accumulation rate is known, the high frequency temperature signal has to have the right timing when the final calculated $\delta^{15}\text{N}$ signal matches the target (or measurement) data. Table 1 contains the final mismatches (2σ) in Δage for all scenarios and shows very well that with a known accumulation rate and firn physics it is possible to fit the Δage history in the Holocene with mean uncertainties better than 2 yr. This table together with a similar statement will be added to the paper in the results section. Figure 2 shows the time series of the mismatches in Δage for all scenarios and is used to clarify the functionality of the algorithm itself.

More interesting for the reviewer is probably the “real world” scenario. Due to the large uncertainties in measured or modelled Δage it is a challenging task to validate the correctness of the Δage regime anyway. But to give an idea to that issue we show here ongoing work. Figure 3 shows the comparison of the Δage regime modelled using our algorithm together with the GISP2 $\delta^{15}\text{N}$ data from Kobashi et al. (2008) and the Δage regime published with the GICC05 GISP2 gas age scale from Seierstad et al. (2014) and Rasmussen et al. (2014). Besides a nearly constant offset of about 20 yr in the early Holocene the agreement is amazing with a standard deviation (2σ) of the mismatches of 7.8 yr over the whole time series and 3.5 yr for the last 8.2 kyr.

For Glacial conditions the task of reconstructing the temperature (with the right frequency and magnitude) without $\delta^{18}\text{O}_{\text{ice}}$ information is much more challenging as mentioned by the reviewer due to the highly variable gas age - ice age differences between stadial and interstadial conditions. Here the Δage can vary several hundreds of years. Also the accumulation rate data is more uncertain than in the Holocene. To prove that the presented fitting algorithm also works for Glacial conditions we inverted the $\delta^{15}\text{N}$ data measured for the NGRIP

ice core by Kindler et al. (2014) for two Dansgaard-Oeschger events, namely DO6 and DO7. Since the magnitudes of those events are higher and the signals are smoother than in the Holocene we only had to use the Monte Carlo type input generator (section 2.4.2) for changing the temperature inputs. To compare our results to the $\delta^{18}\text{O}_{\text{ice}}$ based manually calibration method from Kindler et al. (2014) we used the ss09sea06bm time scale (NGRIP members (2004), Johnsen et al. (2001)) as it was done in the Kindler et al. publication. For the model spin-up we use the accumulation rate and temperature data from Kindler et al. (2014) for the time span 36.2 to 60 kyr. The reconstruction window (containing DO6 and DO7) was set to 32 to 36.2 kyr. As the first guess (starting point) of the reconstruction we used the accumulation rate data for NGRIP from the ss09sea06bm time scale together with a constant temperature of about $-49\text{ }^{\circ}\text{C}$ for this time window. As minimization criterion D for the reconstruction we simply use the sum of the mean squared errors (wRMSE) of the $\delta^{15}\text{N}$ and Δage mismatches weighted with their uncertainties according to the following equation instead of the mean $\delta^{15}\text{N}$ misfit alone as used for the Holocene.

$$D = \sqrt{\text{wRMSE}(\delta^{15}\text{N})} + \sqrt{\text{wRMSE}(\Delta\text{age})} \quad (1)$$

$$= \sqrt{\frac{1}{N} \sum_i \left[\frac{\delta^{15}\text{N}_{\text{meas},i} - \delta^{15}\text{N}_{\text{mod},i}}{\varepsilon_{\delta^{15}\text{N},i}} \right]^2} + \sqrt{\frac{1}{M} \sum_j \left[\frac{\Delta\text{age}_{\text{meas},j} - \Delta\text{age}_{\text{mod},j}}{\varepsilon_{\Delta\text{age},j}} \right]^2}$$

Here $\varepsilon_{\delta^{15}\text{N},i}$ and $\varepsilon_{\Delta\text{age},j}$ are the uncertainties in $\delta^{15}\text{N}$ and Δage for the measured values i or j (Δage match points: Guillevic, M. (2013), p.65, Tab. 3.2) and N , M the number of measurement values. We set $\varepsilon_{\delta^{15}\text{N},i} = 20$ permeg for all i (Kindler et al. 2014) and $\varepsilon_{\Delta\text{age},j} = 50$ yr for all j . The values of 50 yr for the Δage uncertainties were chosen according to reach the same mean relative errors for both terms. The relative uncertainties in Δage can easily reach up to 50% and more in the Glacial using the ss09sea06bm time scale which results in a domination of the $\delta^{15}\text{N}$ misfits over the Δage misfits (10-20% when using GICC05 time scale, pers. communication M. Guillevic). Because of that issue we had to set the Δage uncertainties to 50 yr to make both terms equally important for the fitting algorithm. To sum up: The temperature variations were exactly done in the same way as described in section 2.4.2 within the paper without any further adjustments. We only had to add one target more (Δage) to the minimization criterion to account for a second unknown, i.e. the also uncertain accumulation rates. In fig.4 we show preliminary results. The $\delta^{15}\text{N}$ and Δage fitting (a,b) and the resulting gained temperature and accumulation rate solutions (c,d) using the presented algorithm are completely independent from $\delta^{18}\text{O}$ which provides a great opportunity to evaluate the $\delta^{18}\text{O}$ based reconstruction. In this study the algorithm was used in three steps (MCS0, MCS1, MCS FIN). First, starting with the first guess (constant temperature), the temperature was changed as explained before. The accumulation rate was changed parallel to the temperature allowing a random offset shift (up and down) together with a stretching or compressing (in y direction) of the accumulation rate signal over the whole time window (32 to 36.2 kyr). This first step leads to the ‘‘Monte Carlo Solution 0’’ (MCS0) which provides a first approximation and is the base for the next step. For the next step, we fixed the accumulation rate and let the algorithm only changes the temperature to improve the $\delta^{15}\text{N}$ fit (MSC1). Finally, we allow the algorithm to change the temperature together with the accumulation rate using the Monte Carlo type input generator for both quantities. This also allows the change of the shape of the accumulation rate data. This final step can be seen as a fine tuning of the gained solutions from the steps before. The reached mismatches in $\delta^{15}\text{N}$ and Δage of all steps are at least of the same quality or better than the $\delta^{18}\text{O}$ based manual method from Kindler et al. (2014) (see Tab.2). The gained temperature solutions show a very good agreement in timing and magnitude compared to the reconstruction of Kindler et al. (2014). Also the accumulation rate solutions show that the accumulation has to be reduced significantly compared to the ss09sea06bm data to allow a high quality fit of the $\delta^{15}\text{N}$ and Δage target data, a result highly similar to Kindler et al. (2014) and Guillevic et al. (2013). Regarding the mismatches in $\delta^{15}\text{N}$ and Δage of the final MCS FIN solution show a 15% smaller misfit in $\delta^{15}\text{N}$ (2σ) and an about 31% smaller misfit for Δage (2σ). Keeping in mind that the used approach is completely independent from $\delta^{18}\text{O}$ should clarify the functionality and quality of the presented gas isotope fitting approach also for Glacial reconstructions.

Point (4):

I am surprised the authors don't even attempt to invert the existing GISP2 data (which are even plotted). This seems like a missed opportunity; especially given that it would allow comparison to existing reconstructions to estimate the accuracy of the method.

We understand the surprise of the reviewer of the missing application on existing data but the focus on this paper is indeed the inversion model, its mathematics as well as a proper analysis on the capabilities of the algorithm itself based on a synthetic data set. Yet, we will provide a limited projection on future publications hereafter. However, we underline once more that the accuracy of the inverse modelling algorithm can only be estimated using a synthetic dataset, as shown in our paper. The GISP2 data for $\delta^{15}\text{N}$, $\delta^{40}\text{Ar}$ and $\delta^{15}\text{N}_{\text{excess}}$ are already inverted using the presented algorithm and will be presented in a following publication, since there are a couple of items to be addressed in detail which would overload the scope of the present methodological manuscript. But we want to discuss the algorithm itself to examine what are the possibilities and the limits of the presented fitting method in a well-known modelling framework. The main focus of the present manuscript is to present the algorithm in a single publication rather than in the supplementary to bring the attention on the functionality and fundamental ideas of the algorithm rather than on the gained solutions. We think that is important to give the interested reader the chance to understand the basic concepts behind the algorithm and to show the functionality on a well-known example (here synthetic $\delta^{15}\text{N}$). We hope that we can simplify gas isotope based reconstructions for a broad spectrum of researchers using our or maybe a related approach later on. As we have shown, the approach works for all relevant gas isotope quantities ($\delta^{15}\text{N}$, $\delta^{40}\text{Ar}$, $\delta^{15}\text{N}_{\text{excess}}$) and for Holocene and Glacial data as well. The approach is a completely new method which enables the automatized fitting of gas isotope data without manual tuning of parameters minimizes the “subjective” impact of a single researcher. All together we are sure that this is the best way to present our new elegant fitting method in the framework we have chosen.

Point (5):

The paper is overly long. I recommend section 2.3 be removed entirely, and other sections be shortened considerably. There are also 32 (!) figures in the manuscript, which is too many. Dividing the figures into main, appendix and supplement figures is annoying, as it requires a lot of going back and forth.

We agree that the paper is long and that the amount of figures is possibly too much. This said, we tried to explain and discuss the algorithm in every detail to clarify the functionality of all parts of the fitting method. Our aim was also to present this new method in a totally transparent manner. To shorten the paper we will remove section 2.3 as suggested by the reviewer. This section was thought as a motivation for the presented fitting algorithm. We agree that it is not necessary for the paper itself. Also, we will reduce the numbers of figures by removing the following figures:

Main part: fig01, fig02, fig03

Supplementary: fig.S02 to fig.S16

Next we will shift all the appendix figures in a new supplementary. This means we will have now 4 figures in the manuscript and 11 figures in the supplementary. To keep the paper understandable a further reduction of figures and pages is not possible.

Detailed comments:

Page 1 Line 26: Give references for Holocene temperature reconstructions (there are many!).

Since we developed a novel algorithm for ice core based temperature reconstructions and explained the functionality based on synthetic data of Holocene like behaviour, we gave references to other ice core based reconstruction methods. (borehole inversion, page 1 line 6ff; calibration of water isotopes from the ice core water samples, page 1 line 9ff; $\delta^{15}\text{N}$, $\delta^{40}\text{Ar}$, $\delta^{15}\text{N}_{\text{excess}}$ based methods, page 1 line 14ff). Because no reconstruction for measurement data is shown here, we think it is not necessary to refer for other (or non-ice-core-based) reconstructions.

Page 3 Eq. (1): what about the convective zone? You should correct for that Eq. (2): The surface temperature should really be the temperature at the bottom of the convective zone where diffusion starts to dominate. This may smooth out some of the abrupt decadal-scale temperature variations.

The Schwander model does not use a convective zone at this stage but such a CZ could be implemented in the calculation of $\delta^{15}\text{N}_{\text{grav}}$, by subtracting the gravitational signal formed over the length of the CZ. Has the reviewer examples of a convective zone deep enough to smooth out decadal scale signals except “Megadune” sites (Severinghaus et al., 2010)? We are a bit surprised with this sentence, as for example J. Severinghaus, using measurements from South Pole, shows that already the seasonal signal in gas diffusion affect the first 10 to 12 m of firn (Severinghaus, 1998) pointing to a shallow or even non-existing CZ. Furthermore, we have to remember that we are discussing the rather stable Holocene period in Greenland for which no low accumulation and strong katabatic wind situations are to be expected minimizing the effect of deep CZ. For a CZ to have an effect as strong as to smooth out decadal scale variation, its deepness would need to be of several dozens of meters, which is highly unrealistic even for Glacial Summit conditions. On the contrary the process definitely affecting the damping of the signal is gas diffusion occurring in the firn, producing i) an increase in the mean gas age of the gas at the LID and ii) a damping of the signal whose amplitude is positively correlated with the LID (see for example, Buizert et al. (2012), Fig. 7; Buizert et al. (2013), Fig. 2; and Kindler et al. (2014), Fig. 2).

Line 17: Martinerie et al. (1994) gives the depth of the bubble close-off, whereas $d_{15\text{N}}$ is set at the lock-in depth instead. The LID is shallower than the COD. Is this difference accounted for, and how?

This is explained in details in the description of the Schwander firn model (Schwander, 1997). We did not report details in this paper because we thought this model is a) already quite well known and b) well described in its original paper. However we report this information here: Indeed it is well known that the LID is shallower than the COD, due to the presence of a non-diffusive zone. Originally the COD is defined by a density threshold, calculated as a function of temperature (Marterie et al., 1994). In the Schwander model, to account for the presence of the non-diffusive zone, this COD definition is modified by subtracting 14 kg/m³ to the COD density definition, in order to match the observed depth where gas diffusion stops. This offset was optimised using firn data from Summit (GRIP) collected in the 90', Greenland, and we therefore believe this definition is highly appropriate for the GISP2 site over the Holocene.

Page 4 Section 2.2: what are the model parameters? What are the time and spatial step? How deep does the domain extend? What geothermal heat flux is used, etc.

The model parameters are described in detail in Schwander et al. (1997).

Section 2.3: I recommend this is removed completely. I don't see the point, especially the dynamic case which we know doesn't behave linearly due to memory effects.

To shorten the paper we will remove this section as suggested by the reviewer. This section was thought as a motivation for the presented fitting algorithm. We agree that it is not necessary for the paper itself.

Page 6 Line 13: Not too robust. It'd be easy to have a 10% uncertainty in the thinning function.

We reformulate these sentences from:

“Except for these technical adjustments, the accumulation rate input data remains unmodified, assuming high reliability of this data during the Holocene. This is due to the fact that the data was gained by annual layer counting, and the use of a thinning model which should be rather robust for the first 1500 m of the 3000 m ice core (Cuffey and Clow, 1997).”

The new text now reads:

“Except for these technical adjustments, the accumulation rate input data remains unmodified, assuming high reliability of this data during the Holocene. The data was gained by annual layer counting, and the use of a thinning model which should lead to maximum relative uncertainty of 10% for the first 1500 m of the 3000 m ice core (Cuffey and Clow, 1997).”

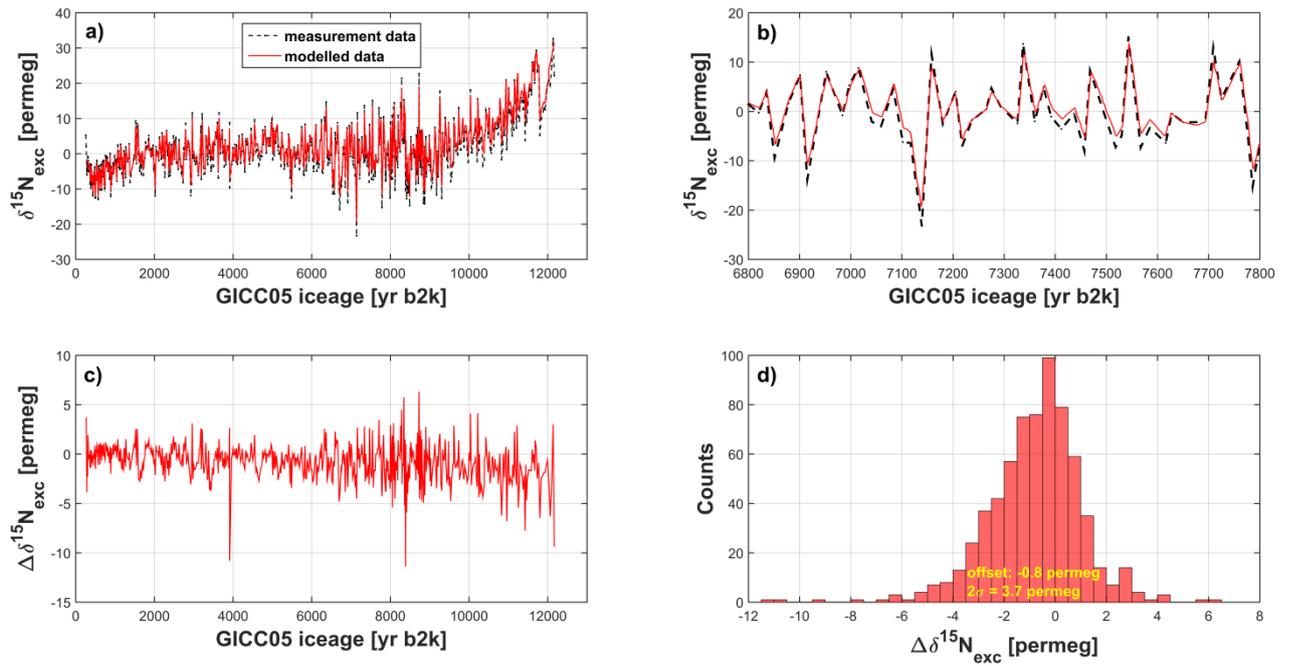


Fig.1: Fitting of GISP2 $\delta^{15}\text{N}_{\text{excess}}$ data (measurement data from Kobashi et al. 2008): a) measured versus modelled $\delta^{15}\text{N}_{\text{excess}}$ time series; b) zoom-in for a randomly chosen 1000 yr interval; c) time series of final mismatches $\Delta\delta^{15}\text{N}_{\text{excess}}$ for the measured minus the modelled $\delta^{15}\text{N}_{\text{excess}}$ data; d) histogram for the same quantity as in c) with values for the final mismatch (2σ) and offset;

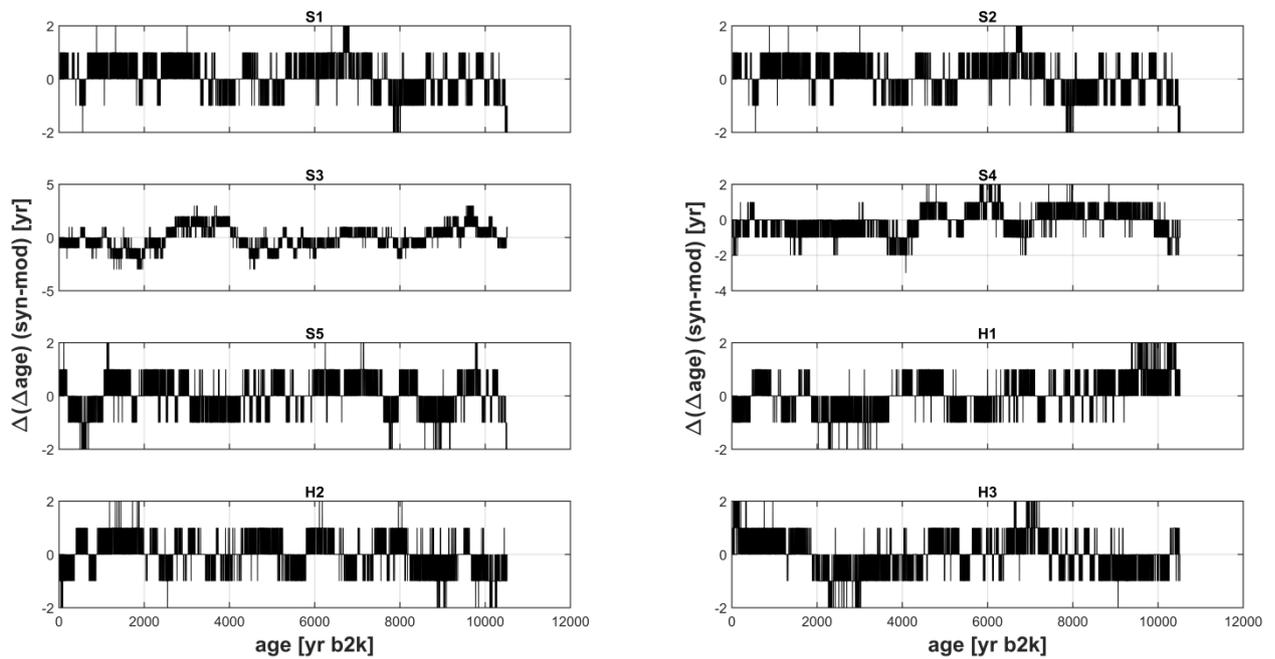


Fig.2: Comparison of the mismatches in Δage between the synthetic target and modelled data for all scenarios showing excellent agreement in Δage . All fits leads to a mean mismatch $\Delta(\Delta\text{age})$ in Δage better than 2yr (2σ).

Scenario:	$2\sigma \Delta(\Delta\text{age})$ [yr]	Scenario:	$2\sigma \Delta(\Delta\text{age})$ [yr]
S1	1.14	S5	1.24
S2	1.60	H1	1.23
S3	1.98	H2	1.18
S4	1.41	H3	1.30

Tab.1: Final mismatches (2σ) of Δage for all scenarios.

Solution	D	Mismatch $\delta^{15}\text{N}$ (2σ) [permeg]	Mean mismatch $\delta^{15}\text{N}^*$ [permeg]	Mismatch Δage (2σ) [yr]	Mean mismatch Δage^* [yr]
Kindler 2014	3.6	44.5	17.9	256	101
first guess	7.8	128.7	63.8	328	138
MCS0	3.1	50.0	19.3	199	82
MCS1	2.9	44.3	17.6	200	84
MCS FIN	2.6	37.8	15.6	175	63

Tab.2: Prove of concept for Glacial reconstruction; *The mean mismatches for $\delta^{15}\text{N}$ and Δage were calculated according to Eq. (7) in the paper.

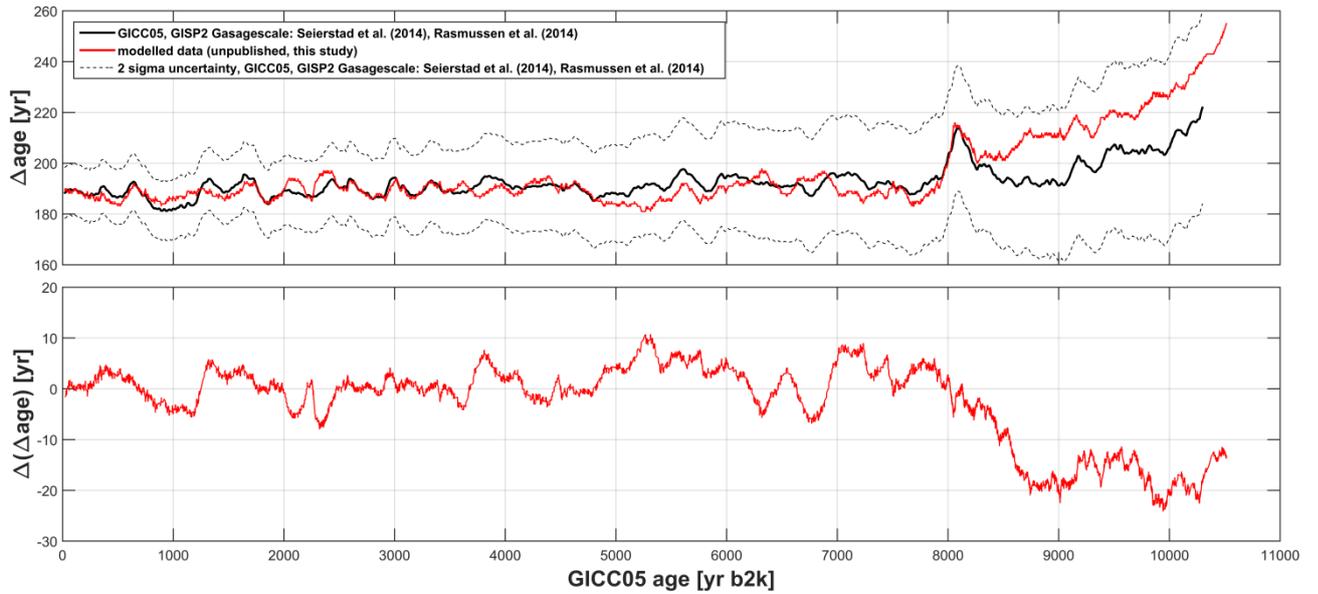


Fig.3: Top plot: Comparison of the modelled Δage (red, unpublished/this study) using the presented approach together with the Schwander model and $\delta^{15}\text{N}$ target data (Kobashi et. all 2008) with the Δage time series for GICC05 GISP2 gasagescale (black curve) from Seierstad et al. (2014), Rasmussen et al. (2014) and related 2σ uncertainty (dotted line). Bottom plot: Time series of the mismatches $\Delta(\Delta\text{age})$ in Δage .

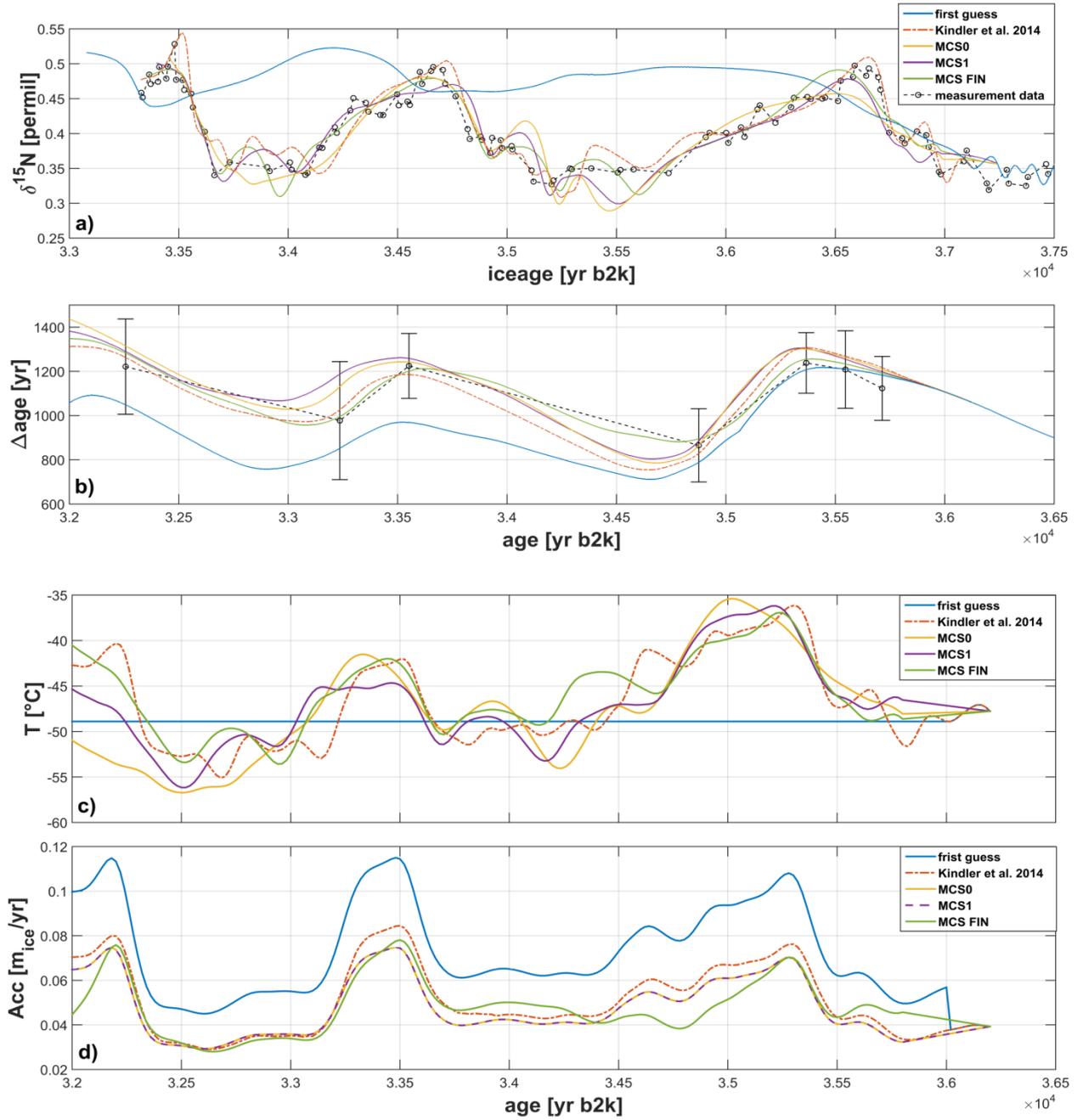


Fig.4: Prove of concept for Glacial reconstructions (NGRIP DO6 and DO7): a) $\delta^{15}\text{N}$ target plot: $\delta^{15}\text{N}$ model output for the first guess input (blue line), Kindler et al. (2014) fit (orange dotted line), Monte Carlo solution 0 (yellow line, unpublished data), Monte Carlo solution 1 (purple line, unpublished data), final Monte Carlo solution (green line, unpublished data), $\delta^{15}\text{N}$ measurement target (black dotted line, measurement points are black cycles, data from Kindler et al. (2014)); b) Δage target plot: Δage model output for the first guess input (blue line), Kindler et al. (2014) fit (orange dotted line), Monte Carlo solution 0 (yellow line, unpublished data), Monte Carlo solution 1 (purple line, unpublished data), final Monte Carlo solution (green line, unpublished data), Δage measurement target (black dotted line, measurement points are black cycles, data from Guillevic (2013)); c) temperature solution plot: first guess input (blue line), Kindler et al. (2014) solution (orange dotted line), Monte Carlo solution 0 (yellow line, unpublished data), Monte Carlo solution 1 (purple line, unpublished data), final Monte Carlo solution (green line, unpublished data); d) accumulation rate solution plot: first guess input (blue line), Kindler et al. (2014) solution (orange dotted line), Monte Carlo solution 0 (yellow line, unpublished data), Monte Carlo solution 1 (purple line, unpublished data), final Monte Carlo solution (green line, unpublished data);

Reply to reviewer 1:

General Comment on reviewer 1:

It was very difficult to find in the comment from reviewer 1 a scientific and/or technical discussion on the scientific questions the presented work is dealing with. This makes it really challenging to find an appropriate way to give an answer on this review. However, we will try to address the key issues and will give an adequate answer in the best possible manner.

This work describes a technical and mathematical variation on previously published work by Kobashi et al. (2010; 2011; 2012).

That is not true at all, which makes us wonder if the reviewer read in detail our submitted article. The presented approach is completely different to the work of Kobashi et al. mentioned here from the reviewer. The calculation of temperature gradients from $\delta^{15}\text{N}_{\text{excess}}$ data used for a temporal integration using the Goujon model as it was done by Kobashi differs from our approach significantly. Our approach calculates in a first step a long term signal in temperature and the isotope target, which is superimposed by a high frequency signal in a next step. Finally we created a correction method for dealing with remaining misfits (permeg level) due to memory effects. Besides the methodology view, we will list 6 major differences between both methods:

- (1) Our approach allows the automated high quality fitting (or inversion) of $\delta^{15}\text{N}$ or $\delta^{40}\text{Ar}$ or $\delta^{15}\text{N}_{\text{excess}}$ data as single targets (as it was mentioned in the paper and shown in the answer to reviewer 2) and provides consequently the opportunity to compare the solution of one target against the others. The method from Kobashi et al. uses all isotope quantities together, eliminating the possibility to compare the reconstruction obtained from one quantity using the other ones.
- (2) Our approach is applicable to Holocene as well as Glacial data (as it was mentioned in the paper and shown in the answer to reviewer 2), whereas the approach of Kobashi et al. was only designed and tested for Holocene reconstructions.
- (3) Our approach allows a parallel adjustment of the accumulation rate input data (if it is necessary) (shown in the answer to reviewer 2 for Glacial data).
- (4) Our approach uses a well-defined minimization criterion which provides the possibility to adapt it to a variety of target combinations (e.g. $\delta^{15}\text{N}$ and Δage for Glacial reconstructions).
- (5) Our approach is not dependent on the choice of the first guess for the reconstruction. A worse choice of this quantity will only elongate the computational time of the “Monte Carlo type input generator” step. This was shown since we used the same first guess (a constant temperature) for all different synthetic data scenarios.
- (6) Our approach splits the reconstructed temperature and isotope signals in a long term and a high frequency signal (for Holocene), which provides additional information and bases for further research questions and uncertainty calculations.

Kobashi et al. innovated by creating a novel hybrid firn densification-thermal diffusion model, much the same as is done here.

To our knowledge, Kobashi et al. used for their reconstruction the already published model from Goujon et al. (2003). The Goujon model is indeed a firn densification model, coupled to an ice sheet flow model also calculating heat transfer from surface to bedrock. The Goujon model does not have a module to automatically optimise the temperature and accumulation scenario needed for the inversion. We agree to this comment in the sense that Kobashi et al. indeed innovated a novel technique to create an input temperature scenario to feed the Goujon model, using firn temperature gradients extracted from $\delta^{15}\text{N}_{\text{excess}}$. We also agree that our approach, similar to the method from Kobashi, needs a firn densification and heat diffusion model to provide the physical basis for the inversion of $\delta^{15}\text{N}$ data. Nevertheless both methods differ significantly from each other as discussed before. Also both methods were created independently.

The scientific advance represented by this work is useful but is very incremental, almost to the point of not standing alone as a publishable scientific paper. It is not clear to me that this work suffices as a "Least Publishable Unit", and reads more like an Appendix to a publication.

We think that this is a very subjective single opinion which is not underpinned by any scientific argument. We created a completely automated algorithm which is able to provide high quality fits for all relevant gas isotope quantities and works as well for Holocene as Glacial conditions. Furthermore the algorithm is not firn model dependent as it was coupled on two state of the art firn models, leading to comparable results. We also refer to the answer on reviewer 2 for point 1, explaining the achievements of this method in detail. Moreover, there are many examples of models presented and published in CP, presenting in details each step of the model, without publishing data related paleoclimate reconstruction alongside. A very well-known example is the recently published automatization method presented by Winstrup et al. (2012) in order to run automated annual layer counting in ice cores using multiple annually resolved records. This paper was very welcomed by the reviewers in CP, and the method has been successfully applied since then to reconstruct chronologies for many ice core records. We believe the focus of our submitted manuscript is very similar to the one from Winstrup et al., applied to a different problem, but always linked to paleoclimate reconstruction.

It would improve the paper if Kobashi's work could be compared to the results found here, and placed in a larger context. Additionally, it would be helpful if the present work were actually used to reconstruct Greenland temperature over the Holocene, much as Kobashi et al. did. I am somewhat surprised that Kobashi is not a co-author, considering how heavily this work relies on Kobashi et al.'s prior work. The synthetic data looks a lot like Kobashi et al.'s actual data. Why not show the actual data?

As explained in detail in the answer on point (4) for reviewer 2, due to the aim of the paper to describe the algorithm in every detail and in a well-known environment (i.e., using a synthetic dataset as target), we decided for not showing the results of the inversion of the GISP2 measurement data within this publication. Also the paper was criticized because of its length and the amount of figures which makes it all together impossible to show everything in a single publication without the danger of losing the scope on the major issues we want to address.

As explained above, our inversion method is entirely new and can therefore not be considered to rely at all on Kobashi's work, which by the way we very much appreciate. However we recognise that obviously our method (as Kobashi's method) works only when coupled to a firm densification model itself coupled to an ice sheet flow model equipped with heat transfer, such as the Schwander or the Goujon model.

Minor comments:

page 1 line 11 "The presented approach is completely automated..."

We correct for that. The new sentence reads:

"The presented approach is completely automated and leads to a match of the $\delta^{15}\text{N}$ target data in the low permeg level and to related temperature deviations of a few tenths of Kelvin for different data scenarios, showing the robustness of the reconstruction method."

page 1 line 23 "since it represents a time of moderate natural variations prior to anthropogenic disturbance, often referred to as a baseline...."

We correct for that. The new sentence reads:

"Holocene climate variability is of key interest to our society, since it represents a time of moderate natural variations prior to anthropogenic disturbance, often referred to as a baseline for today's increasing greenhouse effect driven by mankind."

page 2 line 6 "The studies of Dahl-Jensen et al. (1998) and Cuffey et al. (1995; 1997) demonstrate the usefulness of inverting the measured borehole temperature profile for surface temperature history....."

We correct for that and added the references. The new sentence reads:

"The studies of Dahl-Jensen et al. (1998) and Cuffey et al. (1995; 1997) demonstrate the usefulness of inverting the measured borehole temperature profile for surface temperature history estimates for the investigated drilling site using a coupled heat- and ice-flow model. "

page 2 line 9 "unable to resolve..."

We correct for that. The new sentence reads:

"Because of smoothing effects due to the nature of heat diffusion within an ice sheet, this method is unable to resolve fast temperature oscillations and leads to a rapid reduction of the time resolution towards the past."

page 3 line 24. It is not clear from the wording here which thermal diffusion sensitivity value was used here. Is it the Grachev and Severinghaus (2003), or the Leuenberge et al. (1999)? This must be clarified. A separate issue is that the Leuenberger et al. value is based on measurements that were made in pure nitrogen, not in air. It is well known, and indeed predicted from theory, that the thermal diffusion sensitivity (and thermal diffusion factor) is larger in pure gases than in air. For example, Grachev and Severinghaus measured these parameters in both pure N2 and in air, and found a substantial difference between the two (Figure 1). As can be seen in Figure 1, the thermal diffusion factor in pure N2 is 0.0037 whereas in air it is less than 0.0036. Even more troubling is the fact that the 1960s-era measurements made in pure N2 by the sources that Leuenberger et al. use disagree well outside the analytical error (0.0035) with the pure-N2 value of Grachev and Severinghaus, which was made with a modern mass spectrometer. This suggests that the 1960s era measurements by Boersma-Klein and De Vries (1966) were badly in error. Given the primitive technology of that time, this is not a criticism of these workers, but it is clear that their values should not be used for the present study.

We thank the reviewer a lot for mentioning that point. Indeed we used a wrong equation here, which was a relic from an older version of the paper. We did all calculations using the thermal diffusion sensitivity from Grachev and Severinghaus (2003). We changed Eq. (4) to:

$$\alpha_T = \left(8.656 - \frac{1323 \text{ K}}{\bar{T}} \right) \cdot 10^{-3}$$

page 3 line 26 "The firn model used here behaves purely as a forward model,....."

We correct for that. The new sentence reads:

"The firn model used here behaves purely as a forward model, which means that for the given input time series the output parameters (here finally $\delta^{15}\text{N}_{\text{mod}}(t)$) can be calculated, but it is not easily possible to construct from measured isotope data the related surface temperature or accumulation rate histories."

page 4 line 3 You must say which ice core was used here. Is it GISP2?

We correct for that. The new sentence reads:

"In this study, accumulation rate data from Cuffey and Clow (1997) for the GISP2 ice core, adapted to the GICC05 chronology, is used (Rasmussen et al., 2008; Seierstad et al., 2014)."

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