Bayesian calibration of firn densification models

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10   **Abstract.**

Firn densification modelling is key to understanding ice sheet mass balance, ice sheet surface elevation change, and the age difference between ice and the air in enclosed air bubbles. This has resulted in the development of many firn models, all relying to a certain degree on parameter calibration against observed data. We present a novel Bayesian calibration method for these parameters, and apply it to three existing firn models. Using an extensive dataset of firn cores from Greenland and Antarctica, 15   we reach optimal parameter estimates applicable to both ice sheets. We then use these to simulate firn density and evaluate against independent observations. Our simulations show a significant decrease (25 and 55%) in observation-model discrepancy for two models and a small increase (11%) for the third. As opposed to current methods, the Bayesian framework allows for robust uncertainty analysis related to parameter values. Based on our results, we review some inherent model assumptions and demonstrate how model- and parameter-related uncertainties potentially affect ice sheet mass balance assessments.

1 Introduction

On the Antarctic and Greenland ice sheets (AIS and GrIS), snow falling at the surface progressively compacts into ice, passing through an intermediary stage called firn. The process of firn densification depends on local conditions, primarily the temperature and the snow accumulation rate, and accurate modelling of densification is key to several applications in glaciology. Firstly, variability in firn densification affects altimetry measurements of ice sheet surface elevation changes. 25   Consequently, it is a large contributor of uncertainty in mass balance estimates that rely on a correct conversion from measured volume changes to mass changes (Li and Zwally, 2011; Shepherd et al., 2012; McMillan et al., 2016). Errors in the firn related correction can lead to over- or underestimation of mass changes related to surface processes, and to misinterpreting elevation change signals as changes in mass balance and in ice flow dynamics. Secondly, firn models are used to estimate the partitioning of surface meltwater into runoff off the ice sheet, and refreezing within the firn column, which strongly influences mass loss 30   rates (van den Broeke et al., 2016). Model estimates of current and future surface mass balance of the AIS and GrIS would thus benefit from an improved knowledge of the sensitivity of the densification process to climatic conditions. And finally, the

densification rate determines the firn age at which air bubbles become trapped in the ice matrix. Knowing this age is crucial for precisely linking samples of past atmospheric composition, which are preserved in these bubbles, to paleo-temperature indicators, which come from the water isotopes in the ice (Buizert et al., 2014).

5   Firn densification has been the subject of numerous modelling studies over the last decades (e.g. Herron and Langway, 1980; Goujon et al., 2003; Helsen et al., 2008; Arthern et al., 2010; Ligtenberg et al., 2011; Simonsen et al., 2013; Morris and Wingham, 2014; Kuipers Munneke et al., 2015). However, there is no consensus on the precise formulation that such models should use. Most models adopt a two-stage densification process with the first stage characterising faster densification for firn with density less than a critical value, and then slower densification in the second stage. The firn-model intercomparison of

10 Lundin et al. (2017) demonstrated that, even for idealised simulations, inter-model disagreements are large in both stages. Firn compaction is driven by the pressure exerted by the overlying firn layers. Dry firn densification depends on numerous microphysical mechanisms acting at the scale of individual grains, such as grain-boundary sliding, vapour transport, dislocation creep and lattice diffusion (Maeno and Ebinuma, 1983; Alley, 1987; Wilkinson, 1988). Deriving formulations closely describing the densification of firn at the macroscale as a function of these mechanisms is challenging. Consequently, most

15 models rely on simplified governing formulations that are calibrated to match with observations. The final model formulations have usually been tuned to data either from AIS (Helsen et al., 2008; Arthern et al., 2010; Ligtenberg et al., 2011) or from GrIS (Simonsen et al., 2013; Morris and Wingham, 2014; Kuipers Munneke et al., 2015), consisting of drilled firn cores from which depth-density profiles are measured. However, the calibration of firn densification rates to firn depth-density profiles requires the assumption of a firn layer in steady state. To overcome this limitation, some models have been calibrated against

20 other type of data such as strain rate measurements (Arthern et al., 2010; Morris and Wingham, 2014) or annual layering detected by radar reflection (Simonsen et al., 2013), but such measurements remain scarce and do not extend to firn at great depths below the surface. Ultimately, firn model calibration is an inverse problem that relies on using observational data to infer parameter values.

25 In this study, we adopt a Bayesian approach in order to address firn model calibration. This provides a rigorous mathematical framework for estimating distributions of the model parameters (Aster et al., 2005; Berliner et al., 2008). Bayesian inversion has been applied in several glaciological studies, and it has been demonstrated that this methodology improves our ability to constrain poorly known factors such as basal topography (Gudmundsson, 2006; Raymond and Gudmundsson, 2009; Brinkerhoff et al., 2016a), basal friction coefficients (Gudmundsson, 2006; Berliner et al., 2008; Raymond and Gudmundsson,

30 2009), ice viscosity (Berliner et al., 2008) and the role of the subglacial hydrology systems on ice dynamics (Brinkerhoff et al., 2016b). In the Bayesian framework, model parameters are considered as random variables for which we seek an *a posteriori* probability distribution that captures the probability density over the entire parameter space. This distribution allows not only to identify the most likely parameter combination, but also allows us to set confidence limits on the range of values in each parameter that is statistically reasonable. This enables us to quantify uncertainty in model results, to challenge the assumptions

inherent to the model itself and to assess correlation between different parameters. Calculations rely on Bayes' theorem (see Sect. 2.4 and Eq. (7)), but because of the high-dimensional parameter space and the non-linearity of firn models, solutions cannot be computed in closed form. As such, we apply rigorously designed Monte Carlo methods to approximate the target probability distributions efficiently. By exploiting the complementarity between the Bayesian framework and Monte Carlo
5   techniques, we recalibrate three benchmark firn models and improve our understanding of their associated uncertainty.

2 Data and Methods

2.1 Firn densification data

In order to calibrate three firn densification models, we use observations of firn depth-density profiles from 91 firn cores located in different climatic conditions on both the GrIS (27 cores) and the AIS (64 cores) (Fig. 1). Using cores from both ice
10 sheets is important since we seek parameter sets that are generally-applicable and not location-specific. We only consider dry densification since meltwater refreezing is poorly represented in firn models and wet-firn compaction is absent (Verjans et al., 2019). As such, we select cores from areas with low mean annual melt (<0.006 m w.e. yr^{-1}) but spanning a broad range of annual average temperatures (-55 to -20°C) and accumulation rates (0.02 to 1.06 m w.e. yr^{-1}). For each core, we use the depth-integrated porosity (DIP), also called firn air content. We calculate DIP until 15 m depth ($DIP15$, Eq. (1)). For sufficiently
15 deep measurements, we also calculate $DIPpc$, Eq. (2), taken below 15 m and until pore close-off depth (z_{pc}, where a density of 830 kg m^{-3} is reached). These are the observed quantitative values used for the calibration:

$$DIP15 = \int_0^{15} \frac{\rho_i - \rho}{\rho_i} dz \qquad (1)$$

$$DIPpc = \int_{15}^{z_{pc}} \frac{\rho_i - \rho}{\rho_i} dz \qquad (2)$$

where z (m) increases downwards, ρ is the density of firn (kg m^{-3}) and ρ_i is the density of ice (917 kg m^{-3}). In Eq. (2), we
20 consider porosity only below 15 m to avoid dependency between $DIP15$ and $DIPpc$. We choose to use both $DIP15$ and $DIPpc$ in order to account for first- and second-stage densification. We note that 48 cores are too shallow to reach z_{pc} and so cores which do reach this depth provide a stronger constraint to the Bayesian inference method. This is sensible because these deep cores carry information about both stages of the densification process.

We separate the dataset into calibration data (69 cores) and independent evaluation data (22 cores). The latter is selected semi-
25 randomly; we ensure that it includes a representative ratio of GrIS-AIS cores and that it covers all climatic conditions, including an outlier of the dataset with high accumulation and temperature (see Supplementary Information). The resulting evaluation data has 8 GrIS and 14 AIS cores; 11 of the 22 cores extend to z_{pc}.

2.2 Climate model forcing

At the location of each core, we simulate firn densification under climatic forcing provided by the RACMO2.3p2 regional climate model (RACMO2 hereafter) at 5.5 km horizontal resolution for GrIS (Noël et al., 2019) and 27 km for AIS (van Wessem et al., 2018). Results of the calibration would depend on the particular climate model used for forcing. Each firn model simulation consists of a spin-up by repeating a reference climate until reaching a firn column in equilibrium, which is followed by a transient period until the core-specific date of drilling. The reference climate is taken as the first 20-year period of RACMO2 forcing data (1960-1979 and 1979-1998 for GrIS and AIS respectively). The number of iterations over the reference period depends on the site-specific accumulation rate and mass of the firn column (mass from surface down to z_{pc}). We ensure that the entire firn column is refreshed during the spin-up but fix the minimum and maximum number of iterations to 10 (200 years spin-up) and 50 (1000 years spin-up). We note that at 33 sites, the core was drilled before the last year of the reference climate and so the transient period is effectively a partial iteration of the spin-up period.

In addition to the climatic forcing, another surface boundary condition is the fresh snow density, ρ_0. It is taken as a constant site-specific value. Each value is taken in agreement with the shallow densities measured in the corresponding core of the dataset. We prefer this approach to the use of available parameterisations of ρ_0 (Helsen et al., 2008; Kuipers Munneke et al., 2015) to avoid any error in the fresh snow parameterisation to affect the calibration process.

2.3 Firn densification models

We use the Community Firn Model (Stevens, 2018) as the framework of our study because it incorporates the formulations of all three densification models investigated: HL (Herron and Langway, 1980), Ar (Arthern et al., 2010) and LZ (Li and Zwally, 2011). The Robin hypothesis (Robin, 1958) constitutes the fundamental assumption of HL, Ar and LZ. It states that any fractional decrease of the firn porosity, $\rho/(\rho - \rho_i)$, is proportional to an increment in overburden stress. This translates into densification rates depending on a rate coefficient c, assumed different for stage-1 and stage-2 densification:

$$\begin{cases} \frac{d\rho}{dt} = c_0 \, (\rho_i - \rho), & \rho \leq 550 \; kg \; m^{-3} \\ \frac{d\rho}{dt} = c_1 \, (\rho_i - \rho), & \rho > 550 \; kg \; m^{-3} \end{cases} \tag{3}$$

The formulations of the rate coefficients rely on calibration and thus differ between the three models investigated:

HL

$$\begin{cases} c_0 = \dot{b}^a k_0^* \exp\left(\frac{-E_0}{RT}\right) \\ c_1 = \dot{b}^b k_1^* \exp\left(\frac{-E_1}{RT}\right) \end{cases} \tag{4}$$

Ar

$$\begin{cases} c_0 = \rho_w \dot{b}^\alpha k_0^{Ar} g \exp\left(\frac{-E_c}{RT} + \frac{E_g}{RT_{av}}\right) \\ c_1 = \rho_w \dot{b}^\beta k_1^{Ar} g \exp\left(\frac{-E_c}{RT} + \frac{E_g}{RT_{av}}\right) \end{cases} \tag{5}$$

LZ

$$\begin{cases} c_0 = \beta_0 lz_a (273.15 - T)^{lz_b} \dot{b} \\ c_1 = \beta_1 lz_a (273.15 - T)^{lz_b} \dot{b} \end{cases} \tag{6}$$

$$with \begin{cases} \beta_0 = lz_{11} + lz_{12}\dot{b} + lz_{13}T_{av} \\ \beta_1 = \beta_0 \left(lz_{21} + lz_{22}\dot{b} + lz_{23}T_{av}\right)^{-1} \end{cases}$$

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where $\dot{b}$ is the accumulation rate (m w.e. yr^{-1}), T the temperature (K), T_{av} the annual mean temperature, R the gas constant, g gravity and ρ_w the water density (1000 kg m^{-3}). All remaining terms are model-specific tuning parameters. For $\dot{b}$, we use the mean accumulation rate over the lifetime of each specific firn layer because it better approximates the overburden stress than the annual mean (Li and Zwally, 2011). HL and Ar use Arrhenius relationships with activation energies (E terms) capturing

10   temperature sensitivity and exponents characterising the exponential proportionality of the rate coefficients to the accumulation rate. Originally, Herron and Langway (1980) inferred all values from calibration based on 17 firn cores, from which they inferred the values for the six free parameters (Table 1) of HL. In contrast, Arthern et al. (2010) fixed the accumulation exponents in advance ($\alpha = \beta = 1$) and took activation energies (E_c, E_g) from measurements of microscale mechanisms: Nabarro-Herring creep for E_c and grain-growth for E_g. Still, they noted a mismatch with the activation energy fitting their data

15   best. The k_0^{Ar} and k_1^{Ar} parameters were tuned to three measured time series of strain rates collected in relatively warm and high accumulation locations of AIS. Here, we consider all five $\alpha, \beta, k_0^{Ar}, k_1^{Ar}, E_g$ as free parameters (Table 1) but keep E_c fixed because of its strong correlation with E_g; our use of monthly model time steps and depth-density profiles as calibration data is not suitable for differentiating effects of $\frac{E_g}{RT_{av}}$ and $\frac{E_c}{RT}$. Equation (6) shows that LZ has eight free parameters (Table 1), all denoted by lz in this paper. In contrast to our approach to Ar, we do not add additional accumulation rate exponents to $\dot{b}$ in Eq. (6)

20   because the dependence of c_0 and c_1 on $\dot{b}$ also involves the coefficients lz_{12} and lz_{22} in the definition of β_0 and β_1. Li and Zwally (2011) performed their calibration of Eq. (6) against firn cores only from the GrIS. Later, Li and Zwally (2015) proposed a new parameterisation for β_0 and β_1, but calibrated for Antarctic firn. Since one of the goals of this study is to find a densification formulation applicable to firn in both GrIS and AIS, we choose to apply our calibration method only to Eq. (6) specified in Li and Zwally (2011). However, in our results' analysis (Sect. 3), we also consider the performance of the Li and

25   Zwally (2015) model on the AIS cores of our dataset.

2.4 Bayesian calibration

In our approach, the free parameters of the firn models are identified as the quantities of interest and we define this parameter set as θ. Hereafter, 'original model values' refers to the values originally attributed by Herron and Langway (1980), Arthern et al. (2010) and Li and Zwally (2011) to their respective sets of free parameters θ. The calibration process relies on Bayes' theorem (Eq. (7)) which allows to update a prior probability distribution $P(\theta)$ for θ based on observed data Y.

$$P(\theta|Y) = \frac{P(Y|\theta)P(\theta)}{P(Y)} \tag{7}$$

We use normal and weakly informative priors centred about the original model values so that the constraint of the prior on $P(\theta|Y)$ is minor (Table 1). The data Y consists of the observed $DIP15$ and $DIPpc$ values of the calibration data. The marginal likelihood, $P(Y)$, is a constant term independent of θ and does not influence the calibration. We use a normal likelihood function $P(Y|\theta)$, which quantifies the match of the modelled DIP values with the observed:

$$P(Y|\theta) \propto \exp\left[\frac{-1}{2}(X_{15} - Y_{15})^T \Sigma_{15}^{-1}(X_{15} - Y_{15}) - \frac{1}{2}(X_{pc} - Y_{pc})^T \Sigma_{pc}^{-1}(X_{pc} - Y_{pc})\right] \tag{8}$$

where X_{15} and Y_{15} are vectors containing all modelled and observed values for the calibration data of $DIP15$ respectively, and similarly for X_{pc} and Y_{pc}. We use diagonal covariance matrices Σ_{15} and Σ_{pc} with site-specific variances. The variances determine the spread allowed for the model outputs compared to the observed values and we calculate them taking 5% and 10% margins around $DIP15$ and $DIPpc$ measurements respectively. Allowing for such spread is necessary because multiple causes may lead to model-observation discrepancy such as firn model errors, measurement uncertainties, potential errors in the climatic forcing and approximations in fixing ρ_0. This particular form of the likelihood function assumes independence between model errors in $DIP15$ and in $DIPpc$, which is ensured by our calculation of $DIPpc$ only from 15 m depth to z_{pc} (Eq. (2)). It also assumes normally distributed model errors with respect to the observed values. Both these aspects were verified with preliminary assessments, along with our calculations for the covariance matrices Σ_{15} and Σ_{pc}, as discussed in the Supplementary Information. The posterior distribution $P(\theta|Y)$ gives a probability distribution over the parameter space of a given model conditioned on the calibration data. We note here that extreme parameter combinations in the LZ model can lead to negative densification rates. In such cases, we set the modelled DIP values to 0, which leads to extremely low values for the likelihood and for the posterior probability of such parameter sets.

There is no analytical form of $P(\theta|Y)$ and we must investigate the parameter space to generate an ensemble of θ_i approximating $P(\theta|Y)$. Such an investigation is achieved efficiently using Markov Chain Monte Carlo methods. We apply the well-known Random Walk Metropolis (RWM) algorithm (Hastings, 1970) and summarize it in Fig. 2, on which we base the brief following description. A given model starts with a certain parameter set θ_i and simulates firn profiles at all the calibration sites. Its $DIP15$ and $DIPpc$ results are compared with observations and the general performance of the model using θ_i is quantified by the likelihood. From there and with the prior distributions assumed, the posterior probability $P(\theta_i|Y)$ is computed following Eq.

(7). At this point, the state of the chain is θ_i (Fig. 2a). The RWM then proposes a new θ_i^* from a proposal distribution (Fig. 2b). For the latter, we use the symmetric multivariate normal (MVN) distribution which is centred about θ_i. This implies that the random choice of θ_i^* depends only on the current state θ_i and on the proposal covariance in the MVN, Σ_{prop}, which is discussed below. Using the parameter combination θ_i^*, the model simulates profiles at all calibration sites again (Fig. 2c) and

5    $P(\theta_i^*|Y)$ is computed (Fig. 2d). From there, we either accept or reject the proposed θ_i^* in the ensemble approximating $P(\theta|Y)$. The probability of accepting θ_i^* depends on the ratio $P(\theta_i^*|Y)/P(\theta_i|Y)$ (Fig. 2e). The set saved in the ensemble (Fig. 2g) is θ_i^* if accepted or θ_i if θ_i^* was rejected. The saved set becomes the updated current status for the next iteration θ_{i+1} (Fig. 2a) and the algorithm iterates this process. The RWM has the property that the chain will ultimately converge to a stationary distribution that represents the posterior $P(\theta|Y)$. Thus, after a sufficiently high number of iterations of the algorithm, the

10   ensemble of parameter sets is representative of $P(\theta|Y)$. We verify adequate convergence using a number of tests, which are shown in the Supplementary Information. The proposal variance Σ_{prop} must account for dependence between the different components of θ, i.e. the value of one free parameter can influence the value of another free parameter for the model to reach a good match with the observed data. Σ_{prop} can capture this dependence between parameters and, for optimality, it is updated every given number of iterations (100 in our study) using Eq. (9) (Rosenthal, 2010):

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$$\Sigma_{prop} = \frac{2.38^2}{p} \Sigma_{cov} \tag{9}$$

where Σ_{cov} is the covariance matrix between the free parameters of the model at this stage of the iterative chain and p is the number of free parameters.

From the posterior probability distributions, we can infer the Maximum a Posteriori (MAP) estimates of each model (MAP$_{HL}$,

20   MAP$_{Ar}$, MAP$_{LZ}$). These are the modes of the multi-dimensional distributions over the space of free parameters and have been identified as the most likely sets by the RWM. The MAP estimates can be compared to the corresponding original model values of the parameters. The posterior distributions additionally incorporate the uncertainty in the parameter values. By performing posterior predictive simulations on the evaluation data, we can assess this remaining uncertainty (Gelman et al., 2013). More specifically, we can assume that a large (500) random sample of the ensemble of accepted θ is representative of

25   the posterior distribution. As such, model results computed with all sets of this sample inform about model performance accounting for uncertainty. Intuitively, a large spread in results from a 500 random sample would indicate a large range of possible sets for the free parameters and thus a high uncertainty in parameter values.

3 Results

We present the results of the calibration process after 30000 algorithm iterations and compare the MAP and original models'

30   performances against the 22 evaluation cores. We also evaluate the uncertainty of the posterior distributions and compare performances between the different MAP models.

For both HL and Ar, the posterior distributions for the parameters demonstrate some strong disagreements with the original values (Figs. 3a, 3b). The 95% credible intervals for each parameter incorporate 95% of the marginal probability density in the posterior. Two original parameter values of HL (a, b) and three of Ar (E_g, α, β) lie outside these intervals, and one of HL

5 (k_0^*) is at the lower edge of the interval (Figs. 3a, 3b). This indicates that our analysis provides strong evidence against these original values. The strongest disagreements relate to the accumulation exponents of both models (a, b, α, β). In contrast, the original LZ values agree better with the posterior distribution and all lie within the 95% credible intervals (Fig. 3c).

We use the original models and the MAP estimates to simulate firn profiles at the evaluation sites and we compare DIP results

10 with the observed values. This is an effective way to assess possible improvements in parameter estimates reached through our method since the evaluation sites were not used in the calibration process. The match between observations and the model is improved for MAP_{HL} (Fig. 4a) and even more for MAP_{Ar} (Fig. 4b), with the original Ar strongly underestimating DIP values. These improvements translate into significantly reduced root mean squared errors (RMSE) in modelled values of both $DIP15$ (-26% for HL and -45% for Ar) and $DIPpc$ (-22% and -60%) (Table 2).

15 For LZ, the evaluation against the test set is inconclusive, with a worse performance of the MAP_{LZ} model for $DIPpc$ (+22 % in RMSE) and a slight improvement for $DIP15$ (-1 %) (Table 2 and Fig. 4c). The relative agreement in parameter values between MAP_{LZ} and the original LZ explains more moderate differences in RMSE. Comparing modelled and observed depth-density profiles of evaluation data illustrates the differences in performance visually (e.g. Fig. 5). Profiles of the original models of HL and Ar frequently lie outside the credible intervals of their respective MAP models. In contrast, profiles of

20 MAP_{LZ} and of the original LZ tend to be close together. At the climatic outlier of our evaluation data (DML in Fig. 5), MAP_{LZ} performs slightly worse than the original LZ (Fig. 5i) but improvements are reached for MAP_{HL} and MAP_{Ar} (Figs. 5c, 5f). This demonstrates benefits of this method even at the limits of the calibration range.

Compared to the original HL, MAP_{HL} reaches improvements in $DIP15$ for 12 of the 22 evaluation cores and in $DIPpc$ for 5

25 of the 11 evaluation cores (Fig. 6a). Generally, MAP_{HL} performs better at AIS sites and worse at GrIS sites. An analysis of the improvement of MAP_{HL} as a function of climatic variables (Fig. 6a) shows that the original HL gives better results in a narrow range of T_{av}: from -30 to -25 °C. As such, the better performance at the GrIS evaluation sites is likely due to the original HL being better suited for the particular temperature range corresponding to the conditions of the latter sites. In contrast, MAP_{HL} seems more appropriate for covering a wider range of climatic conditions. For Ar, the original model shows better performance

30 than MAP_{Ar} at few evaluation sites (5 for $DIP15$ and 1 for $DIPpc$) which are only in AIS and confined to low-accumulation conditions (Fig. 6b). This is counterintuitive given that Arthern et al. (2010) tuned the original Ar to measurements from high accumulation sites of AIS. Finally, the original LZ performs better than MAP_{LZ} at most GrIS sites (Fig. 6c), which is unsurprising given that its original calibration was GrIS-specific. Again, this seems related to the original LZ performing

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significantly better in the same narrow range of temperatures as for HL. In total, MAP_{LZ} performs better for 11 of the 22 $DIP15$ and 4 of the 11 $DIPpc$ evaluation measurements.

As explained in Sect. 2.3, the original LZ model was developed for GrIS firn only (Li and Zwally, 2011) and later

5 complemented by an AIS-specific model (Li and Zwally, 2015). Using both of these on the evaluation sites of their respective calibration ice sheet, we construct an LZ dual model, which thus really consists of two different models. The RMSE for $DIP15$ of LZ dual is slightly lower (-9 %) than that of MAP_{LZ} but significantly larger (+37 %) for $DIPpc$. We note that the $DIPpc$ RMSE of LZ dual is strongly affected by the stage-2 densification performing very poorly at the climatic outlier of the evaluation data, with conditions that are outside of the calibration range of Li and Zwally (2015).

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We also compare MAP results with the IMAU firn densification model (IMAU-FDM), which has been used frequently in recent mass balance assessments from altimetry (Pritchard et al., 2012; Babonis et al., 2016; McMillan et al., 2016; Shepherd et al., 2018). IMAU-FDM was developed by adding two tuning parameters to both densification stages of Ar. All four extra-parameters are different for AIS (Ligtenberg et al., 2011) and GrIS (Kuipers Munneke et al., 2015), thus also resulting in two

15 separate models. On the evaluation data, its performance for $DIP15$ is slightly better than MAP_{Ar} and MAP_{LZ} but worse than MAP_{HL}, and its performance for $DIPpc$ is significantly worse than all three MAP models (Table 2).

To assess the uncertainty captured by the Bayesian posterior distributions, we compute results on the evaluation data with the 500 parameter sets randomly selected from each of the three posterior ensembles. For all three models, the average performance

20 of their random sample is similar to the corresponding MAP performance, with a maximum RMSE change of 6% (Table 2). This demonstrates a low uncertainty in the optimal parameter combinations identified by calibration. Furthermore, the best performing 95th percentile of the random selection allows the construction of the uncertainty intervals shown in Figs 4, 5. Of the original models, LZ reaches the lowest RMSE values. MAP_{HL} performs better in both $DIP15$ and $DIPpc$ than any model tested (Table 2). Comparing the performances of MAP models, MAP_{HL} is followed by MAP_{Ar} and then MAP_{LZ}. This order is

25 still valid for the 500-samples random selections, which account for uncertainty (Table 2).

4 Discussion and Implications

This calibration method is potentially applicable to models of similar complexity in a broad range of research fields. We exploit it here to investigate the parameter space of HL, Ar and LZ, and to re-estimate optimal parameter values conditioned on observed calibration data; no further complexity is introduced since the number of empirical parameters remains the same. We

30 treat the accumulation exponents of Ar (α, β) as free parameters whereas Arthern et al. (2010) decided to fix their values to 1. Analogous to a and b in HL, these exponents capture the mathematical relationship between densification rates and the accumulation rate, used as a proxy for load increase on any specific firn layer. No physical argument favours a linear

proportionality between densification and load increase and any prescribed value for these exponents is a choice of the model designer. Unlike Arthern et al. (2010), Herron and Langway (1980) previously inferred $a = 1$ and $b = 0.5$. Our calibration data shows strong evidence against both these pairs of values; all four are outside the posterior 95% credible intervals (Fig. 3a, 3b). Our results of stage-1 exponents (a, α) smaller than 1 indicate a weaker increase in densification rates with pressure. In

5   firn, the load is supported at the contact area between the grains, which increases on average due to grain rearrangement (in stage-1) and grain growth. As such, firn strengthens in time and the actual stress on ice grains increases slower than the total load (Anderson and Benson, 1963). Morris and Wingham (2014) incorporated this by including a temperature-history function, causing slower densification of firn previously exposed to higher temperatures. This is consistent with both grain rearrangement and grain growth because these processes are enhanced at higher temperatures (Alley, 1987; Gow et al., 2004).

10   Lower values of the stage-2 exponents (b, β) illustrate the larger strength of high-density firn with larger contact areas between grains. The same can be applied to the LZ model by investigating the posterior correlation between its free parameters. It shows a positive correlation coefficient (0.6) between the accumulation-related parameters of both stages; lz_{12} and lz_{22}. High values of lz_{12} make β_0 more sensitive to $\dot{b}$ (Eq. (6)). However, β_0 appears in the numerator of the β_1 calculation (Eq. (6)) and higher values of lz_{22} thus moderate the sensitivity of stage-2 densification to $\dot{b}$. As such, positively correlated lz_{12} and lz_{22}

15   provide further evidence that stage-1 densification rates are more sensitive to accumulation rates. The posterior correlations of all three models are further discussed in the Supplementary Information.

HL, Ar and LZ only use temperature and accumulation rates as input variables. Other models use additional variables hypothesised to affect densification rates. These include the temperature-history mentioned above (Morris and Wingham,

20   2014), firn grain size (Arthern et al., 2010), impurity content (Freitag et al., 2013) and a transition region between stage-1 and stage-2 densification (Morris, 2018). Other models are explicitly based on micro-scale deformation mechanisms (Alley, 1987; Arthern and Wingham, 1998; Arnaud et al., 2000). These efforts undoubtedly contribute to progressing towards physically based models. A potential problem with such approaches is overfitting calibration data by adding parameters to model formulations while detailed firn data remain scarce. As long as more firn data is not available to appropriately constrain the

25   role of each variable in model formulations, we favour the use of parsimonious models relying on few input variables. It is noteworthy that MAP$_{LZ}$, which relies on eight free parameters, performs worse on the evaluation data than MAP$_{HL}$ and MAP$_{Ar}$ with two fewer free parameters. This highlights that gains in model accuracy should rely not only on better calibration of parameters but also on a reconsideration of the governing densification equations. Additionally, firn core data invokes the assumption of a steady-state depth-density profile. As such, parameter calibration poorly captures seasonal climatic effects on

30   densification. Comprehensive datasets of depth-density profiles (Koenig and Montgomery, 2019) are very valuable to model development. Efforts in collecting and publishing strain rate measurements from the field (Hawley and Waddington, 2011; Medley et al., 2015; Morris et al., 2017), and possibly from laboratory experiments (Schleef and Löwe, 2013), can further benefit model calibration and the progress towards more representative equations.

As an example of consequences of our calibration, we investigate its effects on GrIS firn thickness change under the 2000-2017 climate. At all 27 GrIS sites of our dataset, we compute the cumulative anomaly in thickness change due to firn compaction during the latter period with respect to the reference 1960-1980 period (see Supplementary Information). Altimetry-based mass balance surveys could interpret any change in firn thickness not captured by firn models as a net gain or

5   loss of ice. The root mean square difference in compaction anomaly between MAP_{HL} and the original HL is 1.5 cm over the 2000-2017 period. If we extrapolate this model-discrepancy to the entire accumulation area of GrIS and convert it to mass, the disagreement between both models corresponds to about 20.6 Gt of ice cumulated over 2000-2017. The same process applied to the original Ar and LZ and their respective MAP yields discrepancies of about 76.6 and 27.4 Gt respectively. Between all six different models, the largest disagreement corresponds to 83.4 Gt, which decreases to 72.1 Gt when considering only MAP

10   models. For reference, we note that the absolute compaction anomaly over the period is equivalent to 870 Gt if averaged across all six models. These discrepancy figures are approximate, since different climatic sensitivities of models and variability in climatic changes will cause compensating effects in different areas. Still, they provide an order of magnitude for potential errors in mass balance assessments that are related to choices of model and of parameter values if firn densification is exposed to a realistic climatic shift.

15   In addition to different cumulative responses, the six models show different sensitivities in terms of monthly values of compaction anomalies over the 2000-2017 period (Fig. 7). Ar shows the strongest sensitivity to climatic conditions diverging from these of the reference period; compaction responds strongly to the general increases in temperature and accumulation rate, especially in late summer. Due to its lower values for α, β and E_g, MAP_{Ar} exhibits less extreme compaction anomalies than the original Ar and thus less seasonal variability. In sharp contrast to Ar, HL-computed compaction rates remain relatively

20   stable, due to low activation energy values that smooth out the seasonal variability. Firn core observations provide little information and constraints on seasonal patterns of densification. However, it is noteworthy that MAP_{Ar} and MAP_{LZ} tend to show comparable short-scale sensitivities (insets in Fig. 7), despite structural differences in the models' governing equations. This might indicate that these models fare relatively well in capturing seasonal fluctuations of densification rates and their sensitivity to climate shifts.

25   **5 Conclusion**

We have implemented a Bayesian calibration method to estimate optimal parameter combinations applicable to GrIS and AIS firn for three benchmark firn densification models (HL, Ar, LZ). An extensive dataset of 91 firn cores was separated into calibration and independent evaluation data. Two optimised models (MAP_{HL}, MAP_{Ar}) showed significant improvement against the evaluation data, while MAP_{LZ} reached results close, but slightly worse, to its original version and inferior to MAP_{HL} and

30   MAP_{Ar}. When compared to other models of greater complexity, the MAP models showed comparable or even improved performances, especially MAP_{HL}. Furthermore, the Bayesian approach provides a robust way to evaluate the uncertainty related to parameter value choice, which is a major deficiency of current models. However, at most sites where we evaluated,

all three models' uncertainty intervals do not cover observed *DIP* values. As such, although model results can be improved by re-calibration methods, model tuning alone is insufficient to reach exact fidelity of firn densification models. The formulation of models' governing equations impacts the remaining errors with respect to observations, which highlights deficiencies in our understanding of dry firn densification. Developing a well-constrained physically detailed model is challenging given the

5   number of mechanisms affecting densification rates and their dependency on microstructural properties of firn, which are difficult to observe. Our study demonstrates that, despite these observational limitations, thorough calibration methods relying only on climatic variables can substantially improve firn model accuracy, and constrain uncertainties.

Author contributions. VV, AL and CN conceived this study. VV performed the development of the calibration method,

10   performed the model experiments and led writing of the manuscript. AL and CN supervised the work. MS developed the Community Firn Model. PKM provided firn core data. BN and JMVW provided the RACMO2 forcing data. All authors provided comments and suggested edits to the manuscript.

Data availability. 41 of the 91 firn cores are from the SUMup dataset (2019 release), which is publicly available from the

15   Arctic Data Center (doi: 10.18739/A26D5PB2S). 41 of the 91 firn cores are from the dataset compiled by Matt Spencer (Spencer et al., 2001), which is publicly available via the NASA Global Change Master Directory as 'LSSU_PSU_Firn_data' (https://drive.google.com/drive/folders/0B_IQfVYZbcWFMDc4M2ZjOTEtNWNhOS00NjdmLTkxMjctYWZlNmZkMDg2 OGFh?hl=en_US). 5 of the 91 firn cores were provided by Joe McConnell and Ellen Mosley-Thompson and are available on request through PKM. 2 of the 91 cores are available via the PANGEA website

20   (https://doi.pangaea.de/10.1594/PANGAEA.227732) and (https://doi.pangaea.de/10.1594/PANGAEA.615238). 1 of the 91 cores is available via the NOAA website (ftp://ftp.ncdc.noaa.gov/pub/data/paleo/icecore/antarctica/newall/). 1 of the 91 cores is available via the USAP website (http://www.usap-dc.org/view/dataset/609215). All Antarctic RACMO2.3p2 climate data used are available on request through JMVW and yearly climate variables are free to download from the IMAU website (https://www.projects.science.uu.nl/iceclimate/publications/data/2018/index.php). All Greenland RACMO2.3p2 climate data

25   used are available on request through BN and yearly SMB and components are free to download (https://doi.pangaea.de/10.1594/PANGAEA.904428). The Community Firn Model is available for download on GitHub (https://github.com/UWGlaciology/CommunityFirnModel).

5 *Competing interests.* The authors declare that they have no conflict of interest.

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| Parameter	Value in original model	Prior distribution	MAP	95 % Credible interval
k_0^* [m w.e.$^{-a}$]	11	$N(11, 25)$	16.3	9.57; 21.84
k_1^* [m w.e.$^{-b}$]	575	$N(575, 2\,10^4)$	627	421; 917
E_0 [J mol^{-1}]	10 160	$N(10160, 1\,10^6)$	10 790	9 660; 11 450
E_1 [J mol^{-1}]	21 400	$N(21400, 4\,10^6)$	21 100	20 200; 21 900
a [/]	1	$N(1, 0.4)$	0.90	0.84; 0.97
b [/]	0.5	$N(0.5, 0.4)$	0.64	0.58; 0.71
k_0^{Ar} [m w.e.$^{-\alpha}$]	0.07	$N(0.07, 1.6\,10^{-3})$	0.084	0.059; 0.154
k_1^{Ar} [m w.e.$^{-\beta}$]	0.03	$N(0.03, 4\,10^{-4})$	0.031	0.020; 0.052
E_c [J mol^{-1}]	60 000	Fixed: 60000	/	/
E_g [J mol^{-1}]	42 400	$N(42400, 25\,10^6)$	40 600	39 500; 41 500
α [/]	1	$N(1, 0.4)$	0.78	0.73; 0.87
β [/]	1	$N(1, 0.4)$	0.70	0.62; 0.74
lz_a	8.36	$N(8.36, 9)$	8.41	4.01; 13.63
lz_b	-2.061	$N(-2.061, 2)$	-2.087	-2.290; -1.913
lz_{11}	-9.788	$N(-9.788, 16)$	-8.962	-17.439; -4.798
lz_{12}	8.996	$N(8.996, 16)$	6.891	4.961; 15.481
lz_{13}	-0.6165	$N(-0.6165, 1)$	-0.6775	-1.258; -0.461
lz_{21}	-2.0178	$N(-2.0178, 2)$	-1.392	-2.394; -0.463
lz_{22}	8.4043	$N(8.4043, 9)$	8.1417	7.030; 12.335
lz_{23}	-0.0932	$N(-0.0932, 0.25)$	-0.0747	-0.100; -0.049

Table 1. Information for the free parameters of HL (top), Ar (middle) and LZ (low). $N(x, y)$ designates a normal distribution of mean x and variance y. The variances in the prior distributions are taken to generate weakly informative distributions. MAP estimates and Credible intervals are results from the calibration process.

| Model	RMSE ($DIP15$) [m]	RMSE ($DIPpc$) [m]
HL original	0.504	2.396
HL MAP	0.371	1.865
HL 500 random sample	0.371	2.135
Ar original	0.770	4.569
Ar MAP	0.425	1.841
Ar 500 random sample	0.430	2.179
LZ original	0.449	1.827
LZ dual	0.398	3.721
LZ MAP	0.446	2.352
LZ 500 random sample	0.473	2.466
IMAU-FDM	0.419	2.681

5 **Table 2.** Model results on the evaluation data. The errors are calculated with respect to the observations of depth integrated porosity until 15 m depth and until pore close-off.
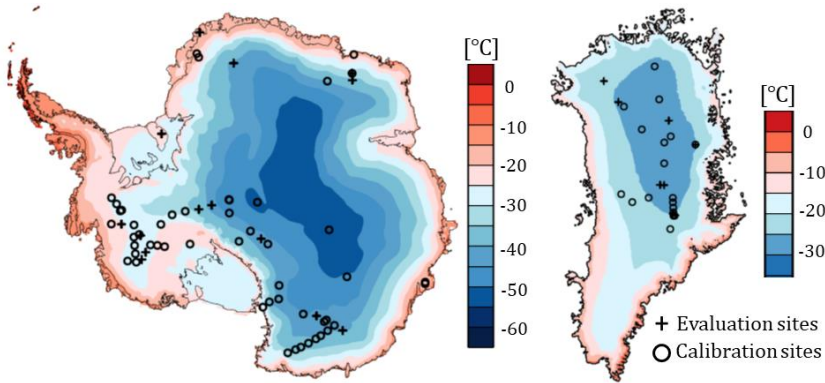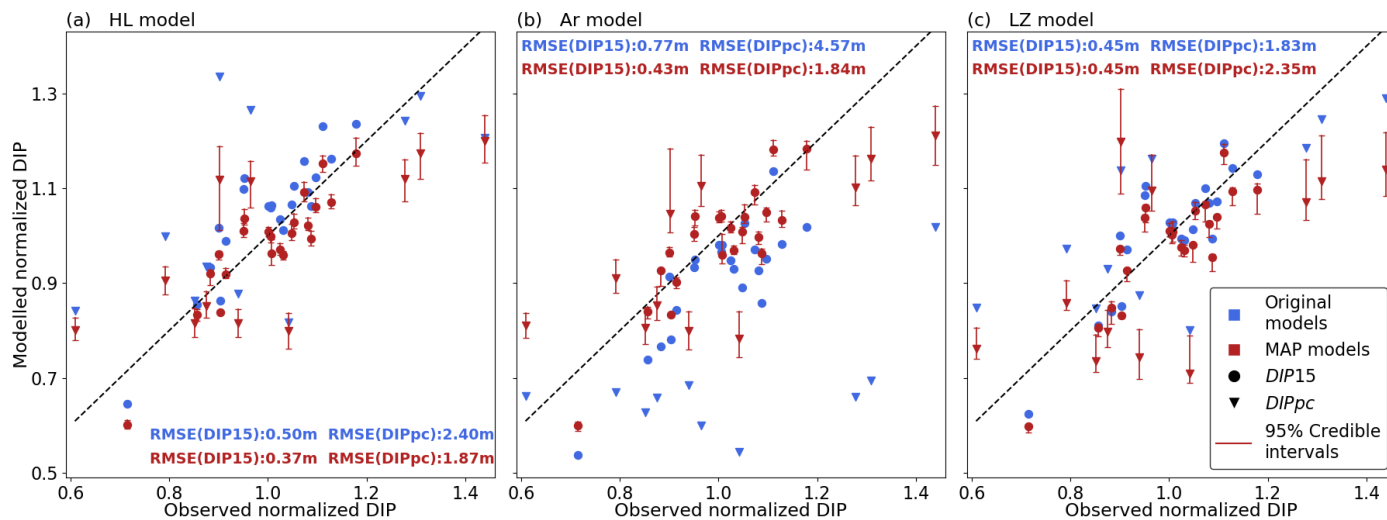
Figure 1. Maps of Antarctic (left) and Greenland (right) ice sheets. Background is mean annual air temperature as modelled by RACMO2.
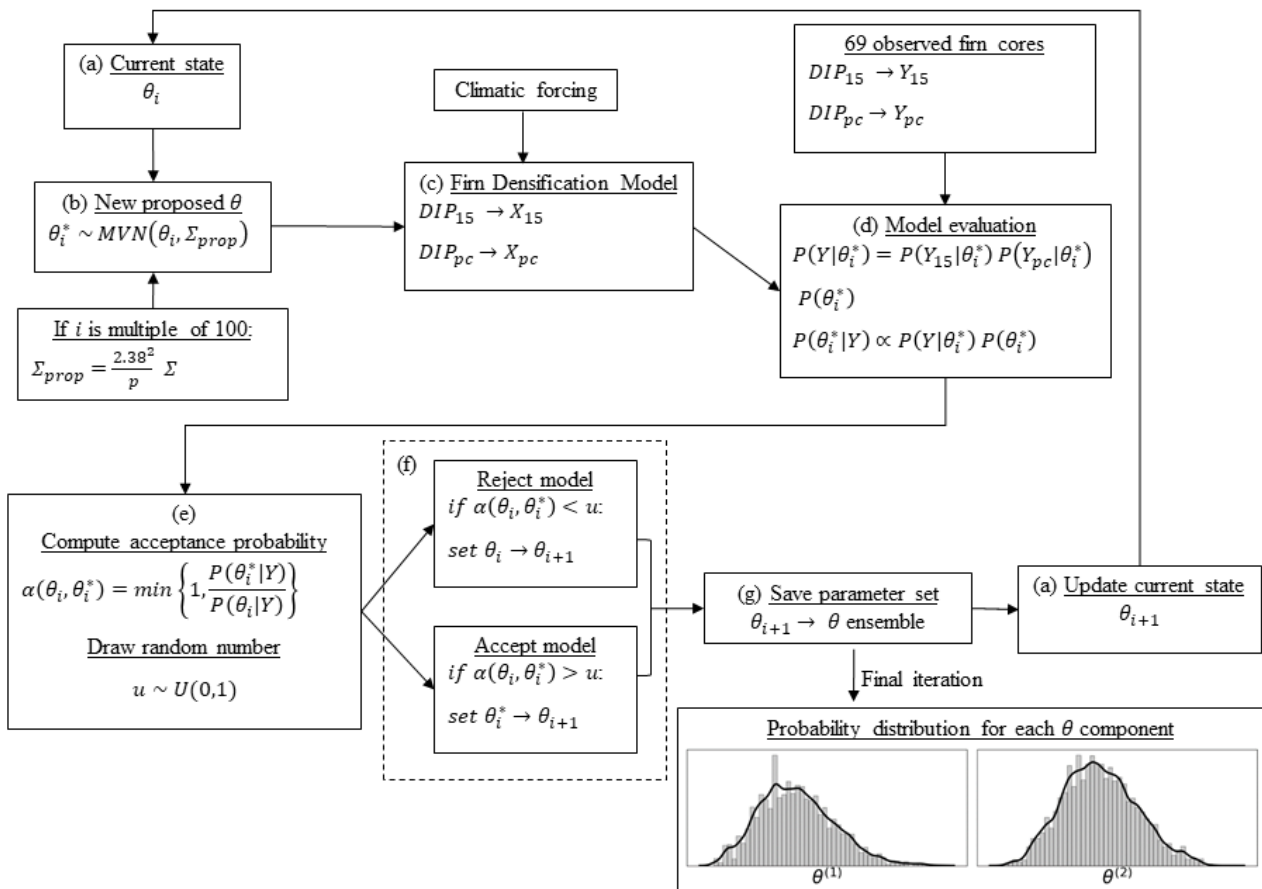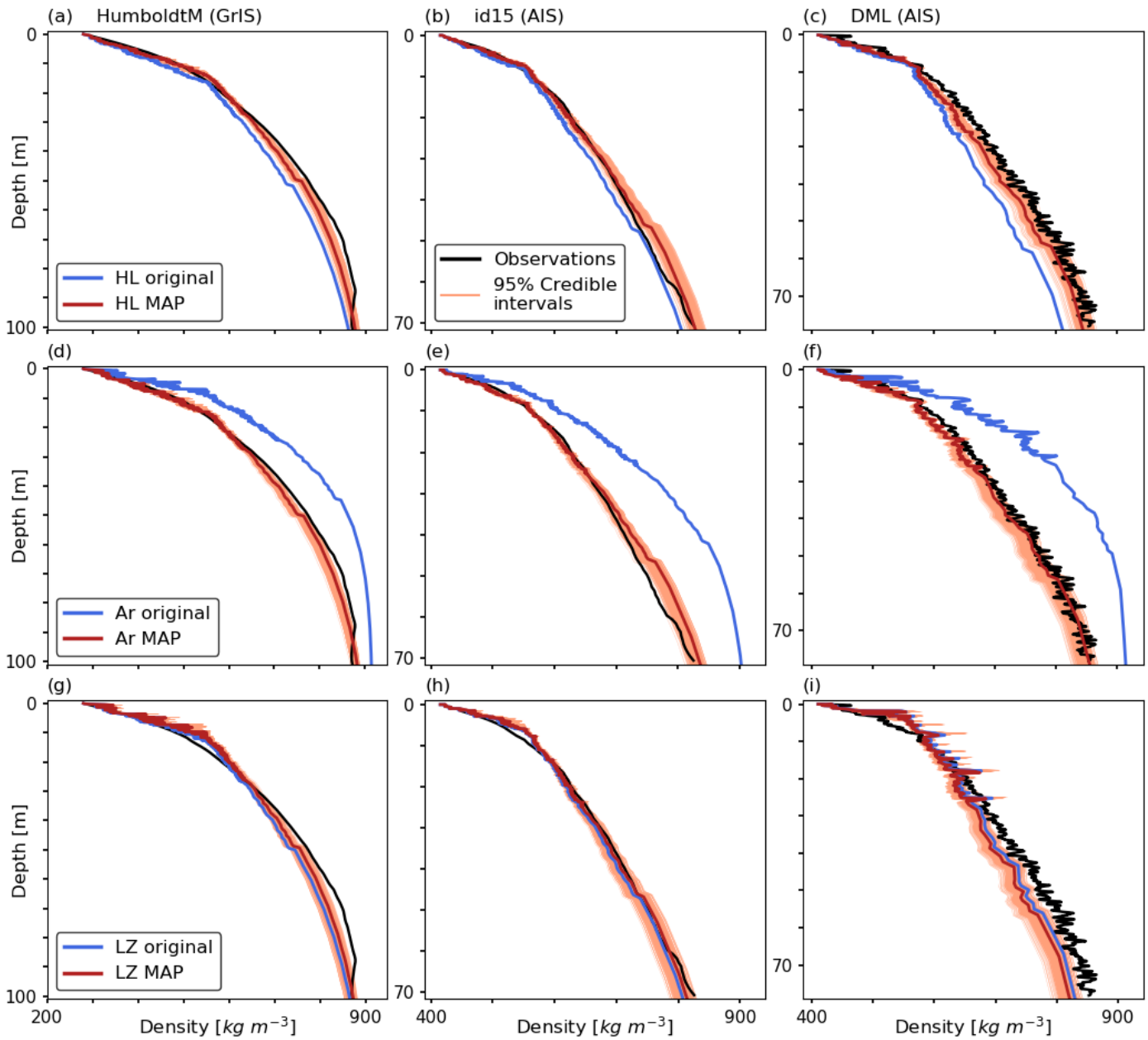

5 **Figure 2.** Implementation of the Random Walk Metropolis algorithm. θ represents a parameter combination of any given firn densification model investigated.
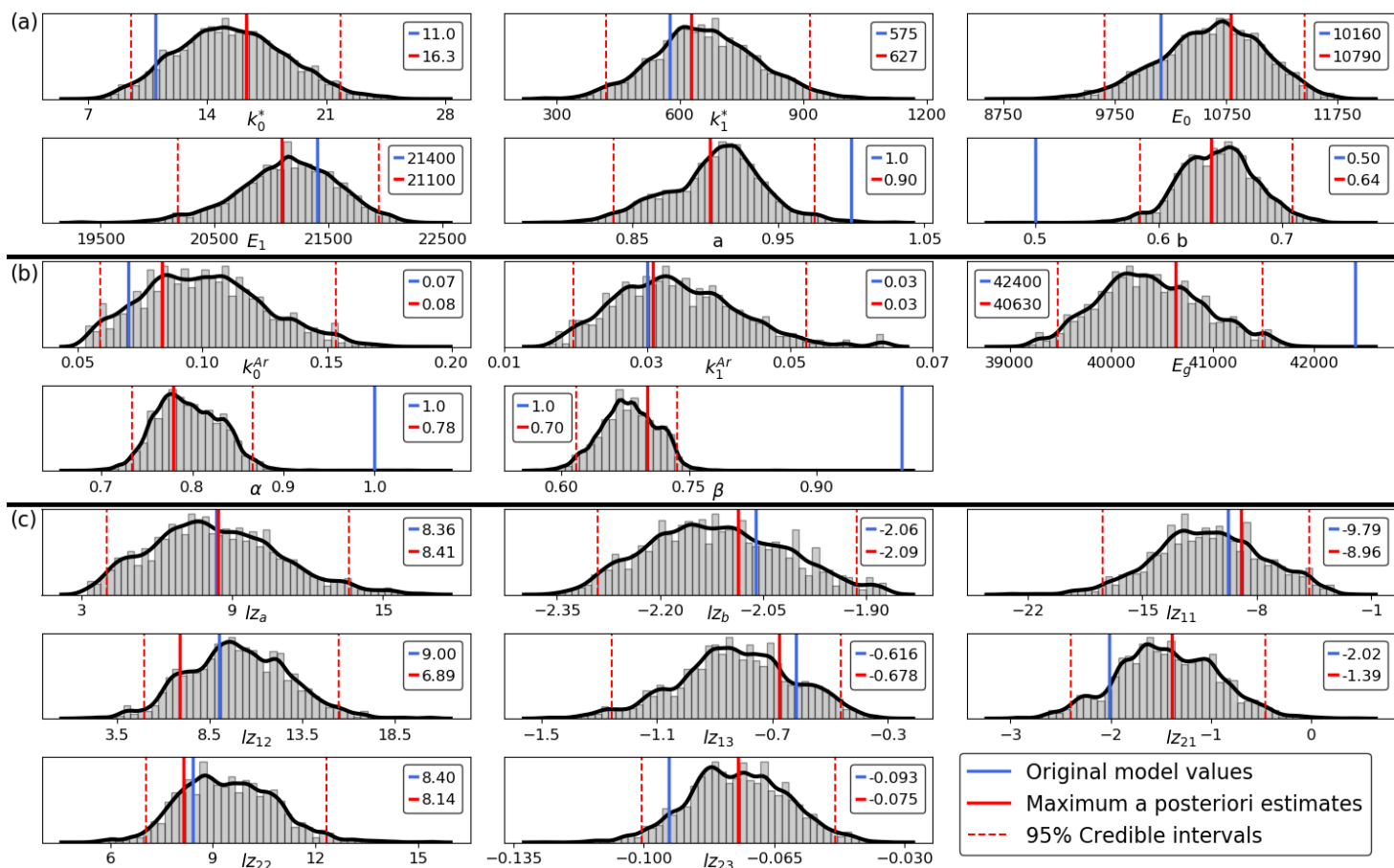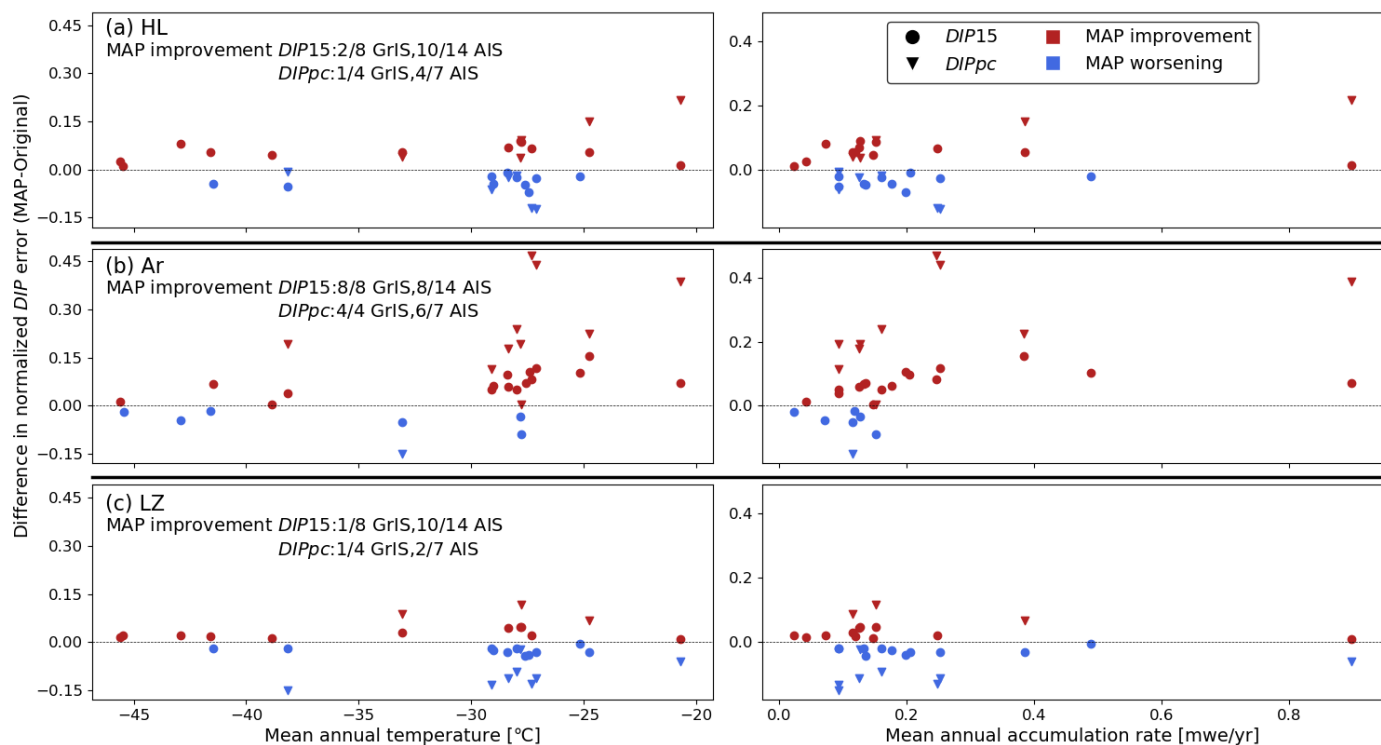
Figure 3. Posterior probability distributions for (a) HL, (b) Ar, (c) LZ.

Figure 4. Comparison of evaluation data *DIP* with model results

Figure 5. Depth-density profiles at three evaluation sites. DMZ is a climatic outlier of our dataset with particularly high temperatures and accumulation rates.

Figure 6. Improvements of the MAP models with respect to the original models for the evaluation data. The ratios indicate the ratios of cores for which an improvement is achieved by the corresponding MAP.
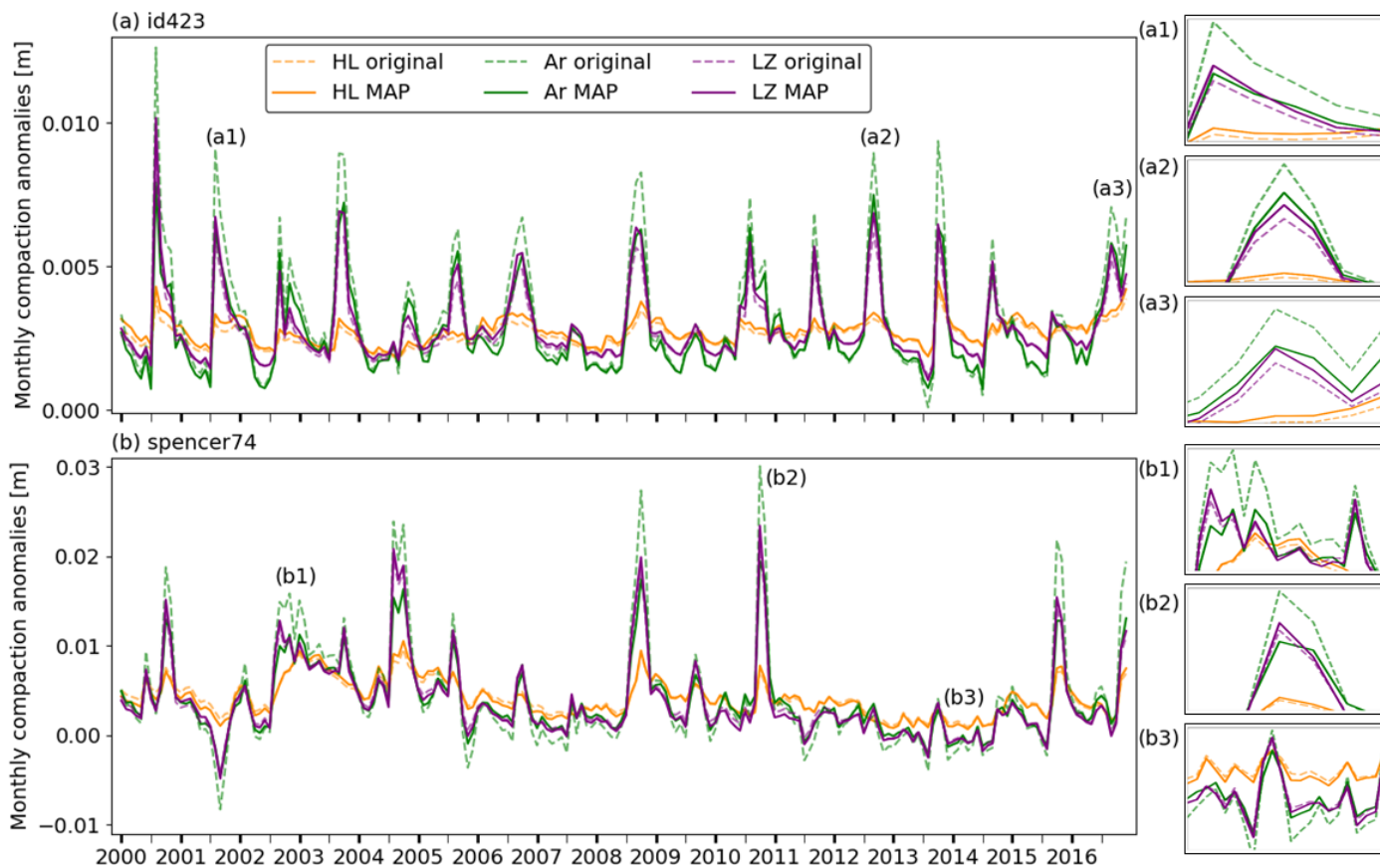
Figure 7. Monthly time-series of compaction anomalies at two sites on the GrIS. Insets show details for particular intervals of the time-series.