

Geostatistical analysis and isoscape of ice core derived water stable isotope records in an Antarctic macro region

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Abstract

Water stable isotopes preserved in ice cores provide essential information about polar precipitation. In the present study, multivariate regression and variogram analyses were conducted on 22 $\delta^2\text{H}$ and 53 $\delta^{18}\text{O}$ records from 60 ice cores covering the second half of the 20th century. Taking the multicollinearity of the explanatory variables into account, as also the

model's adjusted R^2 and its mean absolute error, longitude, elevation and distance from the coast were found to be the main independent geographical driving factors governing the spatial $\delta^{18}\text{O}$ variability of firn/ice in the chosen Antarctic macro region. After diminishing the effects of these factors, using variography, the weights for interpolation with kriging were obtained and the spatial autocorrelation structure of the dataset was revealed. This indicates an average area of influence with a radius of 350 km. This allows the determination of the areas which are as yet not covered by the spatial variability of the existing network of ice cores. Finally, the regional isoscape was obtained for the study area, and this may be considered the first step towards a geostatistically improved isoscape for Antarctica.

Keywords: $\delta^{18}\text{O}$ & $\delta^2\text{H}$ records, isoscape, polar precipitation, variogram analysis

1. Introduction

Due to the increasing interest in the understanding of past global changes, additional and complementary information about past climates is needed. Ice cores play an important role in relation to this issue (EPICA, 2006; NGRIP, 2004; Wolff et al., 2010). For instance, the water stable isotope characteristics stored in them hold crucial information concerning the precipitation they were formed from. The isotopic composition of precipitation, in turn, gives insights into (i) the origin of the water vapor, (ii) the conditions during condensation, and (iii) those during precipitation (Araguás-Araguás et al., 2000; Dansgaard, 1964; Merlivat and Jouzel, 1979). Ice cores can yield information about past climates ranging in time-scale from the seasonal (Hammer, 1989; Kuramoto et al., 2011) up to several hundred millennia (EPICA, 2004), and provide relevant indications about the large-scale dynamics of the Earth's climatic

system (Jouzel, 2013). By integrating the knowledge gained from studying stable isotopes in ice cores into global circulation models, a more detailed picture can be obtained of the climatic factors driving temporal water isotope variability (Werner and Heimann, 2002).

However, dealing with stable isotope data from ice cores in Antarctica is a challenging task, since the spatial availability of cores is sparse and highly variable over the continent (IPICS, 2006; Masson-Delmotte et al., 2008; Steig et al., 2005). Apart from process-based modeling, interpolation is therefore one of the only means available to make estimations between locations for which data are available (Rotschky et al., 2007; Wang et al., 2010).

Interpolated maps representing the global distribution of water stable isotopes in precipitation have been developed (Terzer et al., 2013; van der Veer et al., 2009). These, however, do not cover Antarctica. The only product that maps the spatial distribution of stable isotopic composition in Antarctic surface snow (Wang et al., 2010) neglects the shelf areas. Of these regions, the Filchner-Ronne-, Riiser-Larsen and Fimbul ice shelves cover a fair portion of the area investigated in the present study.

Isoscapes are predictive models that estimate the local isotopic composition of environmental materials as a function of observed local and/or extralocal environmental variables (Bowen, 2010). The horizontal and vertical resolution of isotope enabled global circulation models (GCMs) are steadily improved (e.g. Werner and Heimann (2002); Xi (2014)), such that isotope enabled GCMs using resolutions previously only attainable in regional models are now available (Sjolte et al., 2011; Werner et al., 2011). In the settings where station based precipitation stable isotope records are available, these are naturally the primary inputs to evaluate the performance of isotope enabled circulation models (Lachniet et al., 2016; Sturm et al., 2005). However, gridded products of precipitation stable isotopes (e.g. isoscapes) can be used as additional benchmarks when observations are missing to assess the

global/regional circulation models' effectiveness in replicating observed/interpolated data representing the hydrological cycle and its isotopic counterparts.

The aims of this study were (i) to determine the geographic factors driving the stable isotope variability in a chosen Antarctic macro region; (ii) to assess the spatial continuity properties (variograms) of the stable isotope records, an absolute necessity for geostatistical mapping (Herzfeld, 2004), and (iii) to determine the regional isoscape for ice core derived stable isotope records.

Variogram analysis was used in the hope that it would reveal those areas insufficiently represented by the current set of ice cores, giving an indication of where their spatial coverage might be increased and reveal the spatial dependence structure of the stable isotope records. In addition, variography is vital for kriging (Cressie, 1990; Oliver and Webster, 2014; van der Veer et al., 2009), an "optimal" interpolation which is then employed in the study to estimate the covariances to the highest degree of accuracy possible before mapping. Consequently, the derived isoscape (Bowen, 2010) will be able to describe the spatial distribution of isotopes in the region in a representative way.

Worthy of mention is the fact that the aims of this study are in close agreement with the goals of the International Partnerships in Ice Coring Sciences (IPICS) initiative, since the regional nature of climate and climate forcing requires data from a geographically extensive area. In addition, in order to be able to interpret the water stable isotope records from the past 2 ky of ice cores precisely, these have to be supplemented by additional shorter cores for validation (IPICS, 2006).

2. Materials and methods

2.1. Description of the study area and the used dataset

The Antarctic study area (Latitude (LAT): 71°S, 83°S; Longitude (LON): 61°W, 12°E; Fig. 1) covering about 2.6×10^6 km² in the Atlantic sector, was chosen on account of the relatively high abundance of available ice core derived water stable isotope records, and the fact that it disposes of numerous deep ice cores, which have played and continue to play an important role in paleoclimatology. The region is considered to be diverse from both the topographic and glacio-climatologic perspectives, as well (Graf et al., 1994; Oerter et al., 2000; Rotschky et al., 2007), with areas of low elevation (e.g. the Coastal Dronning Maud Land, Ronne Ice Shelf etc.) at sea level, and significantly higher ones (e.g. the Central Dronning Maud Land > ~2500 m a.s.l.). Field observations have shed light on an atypical continental precipitation distribution obtaining in the region, in which the accumulation and mean air temperature decrease with distance from the shoreline and with the increase in elevation (Vaughan et al., 1999). The difference in accumulation between the highly elevated inland regions and the coast may be as great as a factor of six (Graf et al., 1994; Oerter et al., 2000), and vary by up to e.g. 500 kg m⁻² a⁻¹ over a distance of <3 km in certain areas of the Western Dronning Maud Land (Rotschky et al., 2007); for details see Table S1.

2.2. Dataset used

The data used were acquired from open access data repositories (NOAA (2014); PANGAEA (2014)) and the corresponding research groups (Divine et al., 2009; Naik et al., 2010). Altogether, an array of 22 $\delta^2\text{H}$ (Fig. S1a & b) and 53 $\delta^{18}\text{O}$ (Fig. S1c & d) records was assembled from 60 ice cores spanning various time intervals. In the compiled ice core derived water isotope database, isotope abundances are expressed as per mil (‰), differences from the V-SMOW standard (Coplen, 1994) using the δ notation, $\delta X = [(R_{\text{sample}}/R_{\text{standard}}) - 1] \times 1000$, where X is ²H or ¹⁸O, R_{sample} is the sample ²H/¹H or ¹⁸O/¹⁶O ratio, and R_{standard} is the ²H/¹H or

¹⁸O/¹⁶O ratio of the standard. The longest time interval spanned was almost a millennium (Fig. S1d), while the shortest covered only a couple of years (Fig. S1c).

The study was restricted to the period 1970-1988, corresponding to 44 $\delta^{18}\text{O}$, and from 1970 to 1989 with 22 $\delta^2\text{H}$ records before pre-processing and filtering. In this way, both the time span and the available number of records were maximized. By choosing the higher number of cores against the longer timescale, the possibility of better signal replication arose, as emphasized e.g by Jones et al. (2009). In addition, there were five ice cores (c5, c7, c9, c11 and c13) which only had $\delta^2\text{H}$ records; these were converted to $\delta^{18}\text{O}$ using the regional $\delta^2\text{H}$ - $\delta^{18}\text{O}$ relation established (Fig. S2) based on five neighboring cores with both $\delta^2\text{H}$ and $\delta^{18}\text{O}$ records, (for details see SOM). Note that in one special case, the $\delta^{18}\text{O}$ and $\delta^2\text{H}$ records of two cores spaced only 6 km apart, namely, c48 & c49 NM01C82 _04 (B04) and NM02C02_02 (FB0202) in Schlosser and Oerter (2002) and Fernandoy et al. (2010) respectively were merged together. These are referenced in the present study under code c62 (Fig. S3). In this way, the total numbers of $\delta^{18}\text{O}$ and $\delta^2\text{H}$ records studied using their 1970-1988 averages were 48 and 21 respectively. Reported dating uncertainty of the set of ice cores was $\pm 1\text{yr}$ in both the Dronning Maud Land (Oerter et al., 2000) and the Ronne Ice Shelf (Graf et al., 1999) for the periods closest to the ones assessed in the present study. Therefore, in the case of the $\sim 20\text{yr}$ averages used in the study, dating uncertainty documented above is expected to be negligible.

It is generally acknowledged that the isotopic composition of meteoric precipitation is related to geographical position (Dansgaard, 1964), and can be statistically modeled employing geographical parameters (Bowen and Revenaugh, 2003). These global trends can indeed be generalized to the Antarctic continent (e.g. Wang et al., 2009). On a regional scale, however, the set of independent variables to describe isotope variations may change. In order to be able to analyze the spatial autocorrelation and derive an isoscape of the stable isotope

records, their dependence on geographical factors has to be determined, as in Lorius and Merlivat (1977) or Smith et al. (2002). For the reasons for this and further details, see Section 2.3.

Therefore, in order to determine the geographical factors controlling the ice core water isotopes' variability, latitude (LAT), longitude (LON), elevation (ELE), and distance from the coast (D) were considered in this study. LAT & LON were obtained from the original repository files and converted into meters on a polar stereographic projection with reference to the World Geodetic System 1984 ellipsoid. ELE was extracted from the high-resolution Antarctic digital elevation model (DEM) of Liu et al. (1999), while D was calculated using the shortest perpendicular distances between the sample points representing the ice cores and the coast line.

2.3. Determination of the geographic factors controlling the water stable isotope variability in firn and ice

In order to obtain representative results on the chosen scale from variography, first the effect of the geographical factors controlling the water stable isotopes' variability in fresh and/or metamorphosed snow has to be minimized (Füst and Geiger, 2010; Hohn, 1999). This is because these factors influence the variability of the inspected parameter on a similar and/or larger scale than the phenomena investigated, masking the finer scale pattern, resulting in non-stationarity (Hohn, 1999).

The following procedures refer only to the $\delta^{18}\text{O}$ parameter, because after pre-processing, the number of available $\delta^2\text{H}$ records was found to be too low (for details see Section 3.1). In the case of the Antarctic study area, the spatial/geographic dependence of

precipitation stable isotope composition is well documented (Lorius and Merlivat, 1977; Masson-Delmotte et al., 2008). In the light of these facts, and following the path indicated by previous studies, multiple regression analysis (Draper and Smith, 1981) was chosen to diminish the influence of topography on such first order factors as e.g. condensation temperature and distillation, leaving the effect of the second order factors such as local air mass trajectories and different moisture sources in the residual field.

However, unlike previous studies, multiple factors (e.g. variance inflation, mean absolute error) were taken into account together - as suggested by O'Brien (2007) - to find the best combination of driving parameters.

2.4. Variography

2.4.1. Theoretical background of the semivariogram

The basic function of geostatistics, the variogram, is a tool for describing the spatial autocorrelation structure of the explored variable and to obtain the weights necessary to be able to predict the values of the Antarctic ice core derived $\delta^{18}\text{O}$ annual signal at unsampled locations using kriging techniques (Herzfeld, 2004). The variogram can be described mathematically as follows (Molnár et al., 2010): Let $Z(x)$ and $Z(x+h)$ be the values of a parameter sampled at a planar distance $|h|$ from each other. If samples are taken from the same population (stationarity), and they are in accordance with the intrinsic hypothesis of geostatistics, then the variance (VAR) of the difference of $Z(x)$ and $Z(x+h)$ in a given direction is:

$$\text{VAR} [Z(x+h) - Z(x)] = \text{VAR} [Z(x+h)] + \text{VAR} [Z(x)] - 2\text{COV} [Z(x+h), Z(x)] = 2\gamma(h) \quad (1)$$

The function $2\gamma(h)$ is called the parameter's variogram, while $\gamma(h)$ is its semivariogram and

COV stands for covariance. The semivariogram may be calculated by the Matheron algorithm (Hohn, 1999; Matheron, 1965):

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [Z(x_i) - Z(x_i + h)]^2 \quad (2)$$

where $N(h)$ is the number of lag- h differences, i.e. $n \times (n-1)/2$ and n corresponds to the number of sites. The most important properties of the function (Fig. 2) are: the value C_0 (“nugget”) which withholds information regarding the error of the sampling; the level at which the variogram stabilizes is the sill (C : partial sill + C_0 : nugget) which is equal to the variance for stationary processes, and the range (a) is the distance within which the samples have an influence on each other (Webster and Oliver, 2008) and outside of which they are quasi-independent (Chilès and Delfiner, 2012). This distance (range) determines the average area of influence surrounding the sample locations, within which the measured values of the variable explored are interconnected. In the case of isotropy (Chilès and Delfiner, 2012), the spatial range equals the radius of the area of influence.

If $\gamma(h)$ is a monotonically increasing function (if $h \rightarrow \infty$ then $\gamma(h) \rightarrow \infty$), the parameter is non-stationary (e.g. in Fig. 3). Moreover, if the semivariogram does not have a rising part, the empirical semivariogram’s points will align parallel to the abscissa, giving a nugget-effect type of variogram. In this case, the sampling frequency is insufficient to estimate the range (Hatvani et al., 2014).

Empirical semivariograms by themselves are not yet applicable in spatial modeling. They have to be approximated by theoretical functions in order to provide the necessary weights to be used in kriging (Cressie, 1990) for predicting values at unsampled locations (Chilès and Delfiner, 2012; Herzfeld, 2004). However, a thorough discussion of this question is beyond the scope of the present paper.

From the technical perspective, the variogram analysis was conducted on the residuals of the best multiple regression model of the stable isotope records, with a maximum lag distance set to 600 km and 11 uniform bins about 55 km wide. For further details, please see section 2.3.

2.4.2. Preliminary variography on raw data before minimization of the effect of the geographical factors

Empirical semivariograms were derived from the original/raw data for $\delta^{18}\text{O}$ and $\delta^2\text{H}$. Increasing values of γ were observed for both parameters. For $\delta^{18}\text{O}$ a strictly monotonic pattern; while for $\delta^2\text{H}$, two increasing sections were seen: from the smallest lag distance to ~250 km, then from ~370 km onwards (Fig. 3). It should be noted that in the case of $\delta^{18}\text{O}$ no peaks can be seen as a result of the overwhelming masking effect of geographical factors on water stable isotope variability. Such a variogram cannot be used for further evaluation, as explained in Section 2.4.1. Moreover, in the case of $\delta^2\text{H}$, because of the low number of ice cores (Fig. 1b), γ values could have been calculated for only a few pairs at almost all lag distances (Fig. 3b). Thus, $\delta^2\text{H}$ had to be left out of further analyses.

As discussed in Section 2.3. geographic factors controlling the water stable isotope variability in firn and ice, and their effect has to be minimized. The previous observations on the particular dataset at hand, therefore, further verify the necessity of the minimization of the determining effect of geographic factors controlling the water stable isotope variability in firn and ice before variography can be commenced.

2.5. Isoscape derivation

The procedure of isoscape derivation for the studied Antarctic macro region is based on the methodology used for the global isoscape (Bowen and Wilkinson, 2002) and for an isoscape of an Alpine domain (Kern et al., 2014). The main idea is to:

- (i) create an *initial grid* of the stable isotope variance in the region described by the multiple regression model of the supposedly driving geographic variables (LAT, LON, ELE, D). This step was carried out with the ArcGIS Spatial Analyst Raster Calculator tool;
- (ii) create an interpolated (ordinary point kriging) *residual grid* using the theoretical semivariogram (Section 2.4) fitted on to the residuals of the multivariate regression model; and
- (iii) summarize the corresponding initial (i) and residual (ii) grids to obtain the final map.

Both initial and residual grids were generated uniformly at a resolution of 5 km to facilitate grid calculation. All computations were performed using Golden Software Surfer 11, ArcGIS 10, IBM SPSS 20 and GS+ 10. For certain visualizations of the results, a CorelDRAW Graphics Suite X6 and MS Office 2016 were used.

3. Results

3.1. Minimization of the effect of geographical factors on water stable isotope variability

Motivated by the variogram results on the raw data and the pioneering works of Lorius and Merlivat (1977) and Masson-Delmotte et al. (2008), the geographical factors controlling $\delta^{18}\text{O}$ variability in the region were determined/modeled. The values of the multivariate geographical models were subtracted from the averages of firn/ice $\delta^{18}\text{O}$ records (raw data). In

this way the effects of geographical factors on the averages of firn/ice $\delta^{18}\text{O}$ records for the period 1970-1988 were corrected.

Multivariate regression models were computed and compared using independent variables in various combinations of LAT, LON, ELE and D (SOM Table S2). For example, if LON was omitted, adjusted R^2 (R^2_{adj})=0.98; mean absolute error (MAE) equals 0.87, and a higher degree of multicollinearity was observed than in the case when LAT was omitted. In fact, the latter case was found to be the most robust choice ($p<0.01$) for estimating oxygen isotope variation on geographical parameters, $\delta^{18}\hat{\text{O}}$, (Eq. 3) with an R^2_{adj} =0.98, MAE of 0.95, and an acceptable degree of multicollinearity, which needs to be evaluated in the context of several other factors influencing it (O'Brien, 2007).

$$\delta^{18}\hat{\text{O}} = -(20.51 \pm 0.57) + (2.64 [\pm 0.57] \times 10^{-6}) \times LON - (5 [\pm 0.27] \times 10^{-3}) \times ELE - (1.9 [\pm 0.12] \times 10^{-5}) \times D \quad (3)$$

It should be noted that the uncertainty of the coefficients in the squared brackets is the standard error (SE).

The R^2_{adj} =0.98 may imply that only 2% variance remains in the residuals. However, this is just a method specific and insufficient estimate of the real unexplained spatial variance which is definitely larger (Cressie, 1993). Thus, it has to be explored using variography. The classical non-spatial model (multivariate regression in the present paper) is a special, simplified case of a geostatistical model which is more general (Cressie, 1993). The statistical range of the residuals of the multiple regression spans ~5‰, in addition, their map indicate a spatial structure (Fig. 4a). For instance, negative residuals are observed west of the Berkner Island, or close to zero in Dronning Maud Land and positive ones are clustered south of the

Ronne Ice Shelf. The two ice cores on Berkner Island (c1 & c2) gave two of the most positive residuals. This may be explained by the elevated location of ice cores c1 & c2. It suggests that the regional isotopic altitude effect might be unsatisfactory (too steep) here. The regional isotopic altitude effect is mainly determined by the less depleted $\delta^{18}\text{O}$ compositions, characterized by the low elevated ice-shelf sites and the more depleted compositions characterized by high elevated central Dronning Maud Land. The explanation for these two positive extremes can be that the hills of the Berkner Island are located right at the edge of the ice shelf, but at a relatively higher latitude. The discrepancy suggest that the main physical parameters (arrival temperature, remaining vapor fraction etc.) have a somewhat different effect on the isotopic Rayleigh process compared to the regional average. The strong local influence clearly lead to deviations and the multiple regression model was unable to follow this microregional pattern (Fig. 4a). Thus, ice cores c1 and c2 were left out during variography, but were included in the spatial interpolation step.

3.2. Variography

The empirical semivariogram of the $\delta^{18}\text{O}$ residual was computed with a maximum lag distance set at 600 km, chosen in accordance with the spatial distribution of the cores. The number of cores between 600 and 650 km clearly drops (Fig. S4); as a result, the number of pairs forming the basis of the variogram decreases as well at over ~600 km (Fig. 4b). In addition, with the 55km bins, by keeping the number of pairs relatively even (Fig. 4b) its reliability was ensured. After the empirical variogram was obtained, a best-fit spherical model was determined ($R^2 = 0.72$; residual sum of squares was 0.68) following the protocol strongly recommended by Oliver and Webster (2014).

It is clear that the theoretical variogram is not of the nugget-effect type (for a description, see Section 2.4). After a rising part, it stabilizes at a point just slightly above the variance after reaching the sill (C_0+C), yielding a roughly 350 km spatial range for the average of the 19 years of $\delta^{18}\text{O}$ data used (Fig. 4b). This variogram was later on used to provide the weights for the residual grid derived with ordinary point kriging (Fig. 4c). The standard deviation of the kriging ranged from 0.45 to 1.48 (Fig. 4d). The fact that the kriged map of the residuals (Fig. 4c) reflected a spatial structure and not random noise, clearly indicates that the multivariate regression model was not able to capture this meaningful portion of the spatial variance structure of the firn/ice $\delta^{18}\text{O}$.

3.3. Isoscape derivation for $\delta^{18}\text{O}$

The initial grid was derived employing LON, ELE and D as the main geographical factors driving the $\delta^{18}\text{O}$ variability of firn/ice (Eq 3). The residual grid was modeled using the weights provided by the variogram of the residual $\delta^{18}\text{O}$ (Section 3.2). Afterwards, the initial and residual grids were summed and the regional isoscape of the mean firn/ice $\delta^{18}\text{O}$ was obtained (1970-1988).

The values of the residual grid varied by up to 11.8% of the initial grid (Fig. S5), containing a fair portion of the spatial variance of the snow/firn $\delta^{18}\text{O}$. Thus, if the residual grid had not been taken into account, this would have been lost. With the average spatial range, the area of influence can then be plotted and unified for the set of examined ice cores. This union indicates the areas where the spatial model is reliable from the geostatistical point of view (Fig. 5), while the map of the standard error of kriging offers an alternative measure of the accuracy of the derived $\delta^{18}\text{O}$ isoscape (Fig. 4c).

4. Discussion

4.1. Dependence on geographical factors

Since the main aim of the present study was to determine the spatial range using variography, the effect of the regional geographical factors on firn/ice $\delta^{18}\text{O}$ variability had to be minimized. For decades, scientists have been keenly studying the relationship between geographical factors and the stable water isotope composition of surface snow and firn in Antarctica both on a continental and a regional scale, for example Lorius and Merlivat (1977) and the others as may be seen in Table 1.

In regional studies, the number of independent variables applied has in general been smaller than in the present case. In certain Antarctic macro regions the set of geographical factors governing the distribution of stable water isotopes has mainly been determined by elevation (Altnau et al., 2015; Smith et al., 2002). It should be emphasized that in the present case LON, ELE & D explained 98% of the variance in the area explored, just as in the work of Altnau et al. (2015), which overlapped with a fair portion of the western part of our studied region.

In general the explanatory power of the models in these studies was lower than those used here, and although there were cases when multiple criteria were used to evaluate the models (Wang et al., 2010), this was not the most common practice. Usually R^2 was used (e.g. Altnau et al. (2015); Masson-Delmotte et al. (2008)), and despite its importance (O'Brien, 2007), no attention was paid to multicollinearity, unlike in the present study. In addition, the data gathered here were homogeneous, inasmuch as firn/ice core data uniformly averaged for 1970-1988 were used. Casual snow samples or averages of hundreds of meters of ice cores were omitted to avoid potential bias towards a short or extraordinarily long time frame. These

considerations make the presented approach more reliable for the region than any other previously.

A comparison with previous studies partially overlapping in time and/or space on the dependence of these geographical factors led to meaningful results only in the case of elevation. The value of 0.005 ‰ m^{-1} obtained in the present study was of the same order as those in the literature, but was one of the lowest among them even if uncertainty (SE in Eq. 3) is taken into consideration. In particular, for the investigation of areas ranging between the coastline and the East Antarctic Plateau (Altnau et al., 2015; Smith et al., 2002), the coefficient of elevation (0.008 ‰ m^{-1}) was higher than that in the present study. For research conducted on a continental scale, the derived coefficients have been lower (0.007 ‰ m^{-1} Masson-Delmotte et al. (2008) and 0.0068 ‰ m^{-1} (Wang et al., 2010)). Our lower value can be explained by the fact that only a small part of the area investigated here extends onto the East Antarctic Plateau where a steeper elevation effect was observed.

The two most outlying model residuals suggested that the multivariate regression applied here was unable accurately to capture the microregional characteristics of the elevated relief of Berkner Island (c1 & c2) rising between the Ronne and Filchner Ice Shelves (Fig. 1). These regional differences lead to the omission of ice cores c1 and c2 from the multiple regression model.

On the basis of the results presented here, it may be suspected that on the scale of the investigated region LON, distance from the coast (D) and elevation (ELE) are accounted as determining most of the variance of $\delta^{18}\text{O}$ attributable to geographical factors in the area. This makes sense, since, from a physical point of view, elevation is a main determinant of condensation temperature. The distance from coast controls moisture loss efficiency related to sequential precipitation events on the course of the inland transport of the air parcel.

However, these factors do not fully account for second-order controls e.g. specific local air mass trajectories, the differing seasonality of moisture sources for precipitation in Antarctica (Sodemann and Stohl, 2009). By removing the driving effect of the geographical (first order) factors with Eq. 3, the net effect of the previously mentioned second order factors (see section 2.3) was retained in the residuals. These ultimately provided the input values for the variography and consequently the residual grid when the isoscape was modeled.

4.2. Variography and isoscape derivation

4.2.1. Variography and kriging

After the governing effect of geographical factors on firn/ice $\delta^{18}\text{O}$ variability had been minimized, the dataset was prepared for variography. In contrast to mathematical interpolation, where the same algorithm is applied to every location, geostatistical interpolation using variograms is able to take regional properties into account (Herzfeld, 2004). It provides a spatially more data adaptive approach as underlined by Wang et al. (2010) in his research on water stable isotopes.

The statistical uncertainty of the interpolation may come from variography: the nugget ($\sqrt{C_0} = 0.36\text{‰}$) referring to the sampling error and the kriging standard deviation (KSD; higher than 0.45‰ ; Fig. 4c) are governed by the spatial distribution of the ice cores (Chilès and Delfiner, 2012). In an ideal case, exact interpolation is indicated by KSD being zero (Wackernagel, 2003), which is anyhow unlikely in nature. If $C_0 > 0$, as in the present case (Fig. 4a), this was impossible. These uncertainties were acceptable, since the usual analytical accuracy of the stable oxygen isotope analysis is $\sim 0.1\text{--}0.2\text{‰}$ depending on the applied isotope analytical method (Lis et al., 2008). In addition, the well-known stratigraphic noise as a

natural factor in ice core records (Fisher et al., 1985) also affected the firm $\delta^{18}\text{O}$, causing signal disturbance over small distances.

4.2.2. On isoscape and spatial range

The presented $\delta^{18}\text{O}$ isoscape describes an Antarctic macro region, 20% of which ($\sim 0.5 \times 10^6 \text{ km}^2$) lies on ice shelves (Scambos et al., 2007). Oddly, it is not covered by the continental $\delta^{18}\text{O}$ maps, despite the existence of data (Wang et al., 2009, 2010). As expected, the mean stable isotope content indicated by the isoscape (Fig. 5) decreased with increasing elevation & distance, and with temperatures decreasing inland. These phenomena can be explained by isotopic fractionation inducing the preferential condensation of heavier isotopologues during precipitation processes, leading to depleted water stable isotope composition for both water vapor and precipitations penetrating the continent.

Ambient temperature is a primary physical factor in determining $\delta^{18}\text{O}$ variability in precipitation and therefore also influences surface snow and consequently firm/ice isotope variability. Thus, it was interesting to compare the spatial characteristics of $\delta^{18}\text{O}$ in surface snow and temperature. Unfortunately, due to the lack of comparable direct instrumental temperature measurements in space and time for such purposes, monthly mean near surface (2 m) air temperature, representing the region of interest from 1970 to 1988 had to be used. This data was extracted from NCEP/NCAR Reanalysis Products (Kalnay et al., 1996). The same data treatment was applied for the temperature field as for the $\delta^{18}\text{O}$ records of the ice cores, and variography was conducted on the residuals of its multiple regression model (Table S3). The spatial range of the temperatures at the near surface- (2 m) was 428 km (Fig. 6).

It is well-known that the inversion and surface temperature are well correlated in Antarctica (Jouzel et al., 1987), exhibiting a gradient of 0.67 for correspondent temperature changes with changes at the surface being larger. Therefore, a positive correlation between water isotope composition and surface temperature is expected.

A recent field study (Steen-Larsen et al., 2014) documented in the upper most 0.5 cm of snow an imprint of the isotopic composition of vapor, by vapor exchange even between precipitation events pointing to the imprint of ambient temperature variations via fractionation processes. This surface processes can modify the temperature signal imprinted into the stable water isotopes transported to the surface by precipitation from the cloud formation level. This is further supported by the statistical evidence of related data (Hatvani and Kern, 2017). The similar spatial variability domains for firn/ice $\delta^{18}\text{O}$ (350 km) and for the near surface temperature (428 km) might be an indication that most of the observed water isotope variations are temperature driven, yet the shorter domain for $\delta^{18}\text{O}$ calls for additional factors to be involved.

Indeed, other phenomena, such as post deposition processes (e.g. stratigraphic noise (Fisher et al., 1985)), can be also considered as major factors in the determination of $\delta^{18}\text{O}$ variability. It is interesting to note that a variogram analysis of surface snow accumulation in an area overlapping with the domain of the present study reported the effective radii of spatial autocorrelation to be 200-250 km from NE to SW and 100-150 km perpendicular to this direction (Rotschky et al., 2007). The previously mentioned stratigraphic noise is therefore a major factor in driving the spatial variability of snow accumulation.

Thus, the intermediate “position” of the firn/ice $\delta^{18}\text{O}$ spatial range between the ranges characterizing the spatial variability of air temperature and snow accumulation reinforces the notion that a combination of these processes is responsible for firn/ice $\delta^{18}\text{O}$ spatial variability.

4.2.3. A practical message for future site selection

If the aim is to study spatial (from regional to continental) variations of ice/firn stable isotopes one or two drilling sites are unsatisfactory. Therefore, in the case of an array of ice cores geostatistical planning is inevitable to optimize sampling, as done in the case of the International Trans-Antarctic Scientific Expedition (Cressie, 1998). In the presented region of Antarctica, the 350 km spatial range conveys the clear message that the current set of ice cores does not cover the whole sector. The area outside the coverage of the cores (outside the union of the range ellipses (Fig. 5)) is where new ice cores can contribute the most to the ice core network as an additional geostatistical criterion for optimal site selection (Vance et al., 2016). The drilling of additional cores would be helpful in the improvement of the description of spatial variability, as has also been suggested by the IPICS (2006) initiative. If samples are taken by interpolation in the areas outside the range ellipses' union, the interdependence structure of firn/ice $\delta^{18}\text{O}$ variability remains undetectable, as samples there are already quasi-independent (Chilès and Delfiner, 2012). Naturally, if new cores are drilled, it may be presumed that the spatial autocorrelation structure of the dataset will change, and therefore after any such campaign, a recalibration would be required.

5. Conclusions

Using the obtained dataset, the regional dependence of firn/ice $\delta^{18}\text{O}$ variability on geographical factors was determined. It was shown that (i) in the study area $\delta^{18}\text{O}$ variance was most precisely estimated - taking multicollinearity into account as well - by employing longitude, elevation and the distance from the coast in a multivariate regression model.

Consequently, after correction for the effect of the geographic influence, the spatial autocorrelation structure was revealed using variography, serving as the basis for isoscape derivation employing kriging. The 350 km spatial range explicitly indicates the areas not as yet covered by the currently available network of ice cores. Furthermore, the geostatistical findings support the notion that the combination of the spatial variability of air temperature and snow accumulation is likely to regulate firn/ice $\delta^{18}\text{O}$ spatial variability. These results bring us closer to the accomplishment of one of the ultimate aims of research in this field, an improved continental isoscape for Antarctica, since it has so far been neglected in global isoscapes (Terzer et al., 2013; van der Veer et al., 2009).

Furthermore, we provide additional information about the spatial extent of a common water stable isotope signal in Antarctica and offer guidance to experimenters on where to drill additional cores in order to improve the overall representativeness of the shallow Antarctic ice/firn core network. Moreover, the derived isoscape can be used as a benchmark in model validation of isotope enabled GCMs in the case of scarce station based precipitation stable isotope records over Antarctica.

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Figure captions

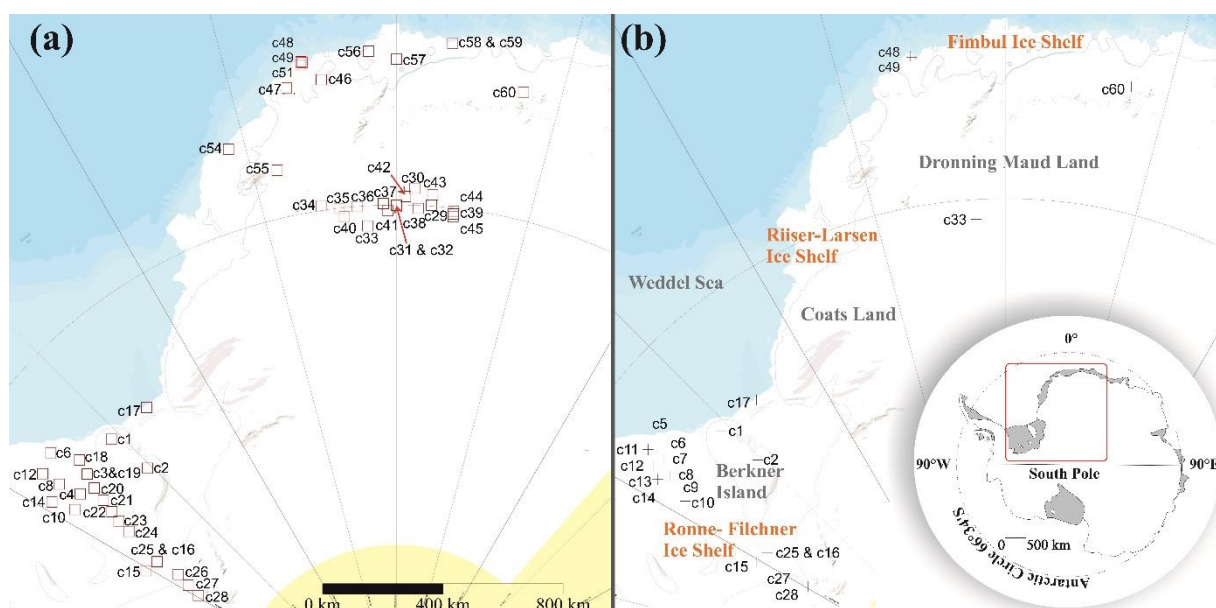


Fig. 1. Spatial distribution of the analyzed (a) $\delta^{18}\text{O}$ and (b) $\delta^2\text{H}$ ice core records. The study area is marked by a red rectangle on the inset map (bottom right)

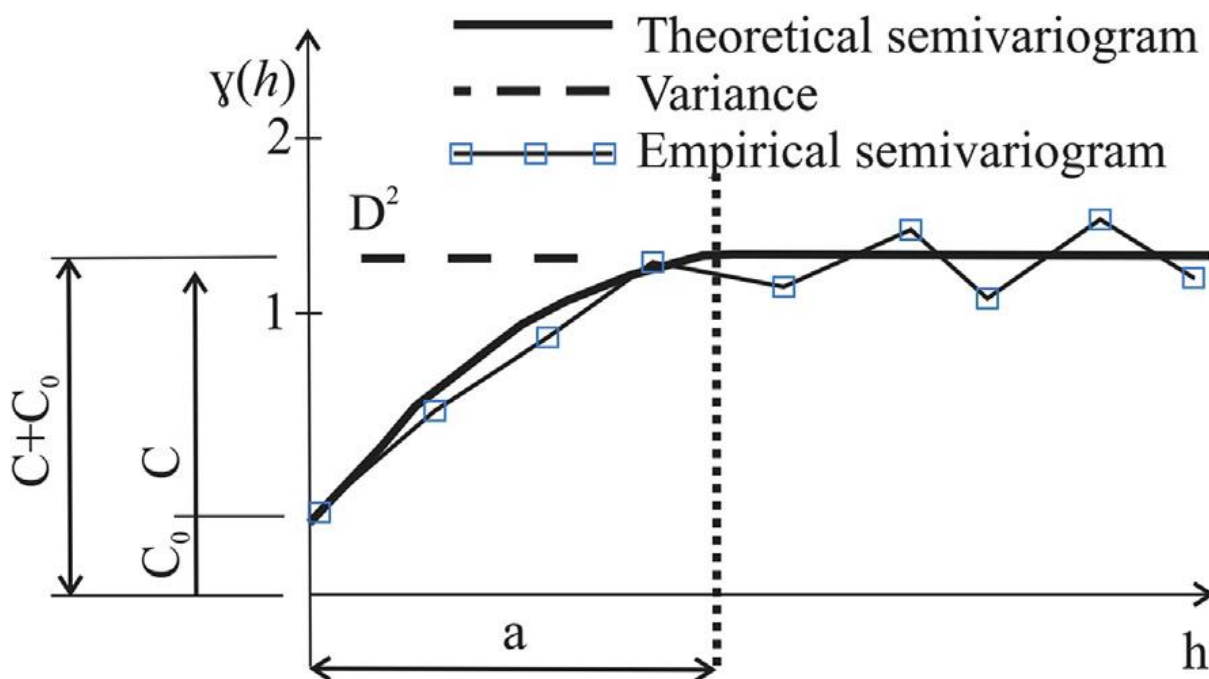


Fig. 2. Properties of the semivariogram, where “a” stands for the range, “C” for the reduced sill and “C0” for the nugget, if $C_0 > 0$, “h” for lag distance, and “ D^2 ” for the variance of the whole investigated data set; based on Füst and Geiger (2010)

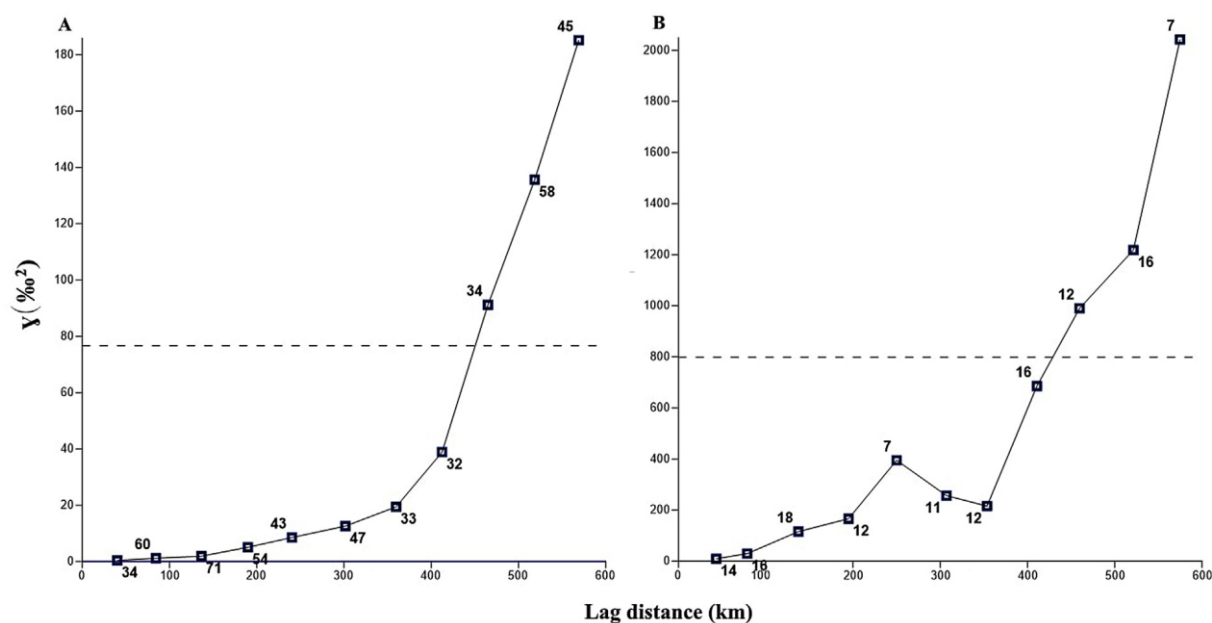


Fig. 3. (a) Empirical semivariogram (squares) derived from the mean original and (1970-1988) $\delta^{18}\text{O}$ and (b) (1970-1989) $\delta^2\text{H}$ values, with the broken line indicating the variance. The numbers indicate the number of data pairs that were used to derive the variogram value for a particular bin; bin widths were 55 km.

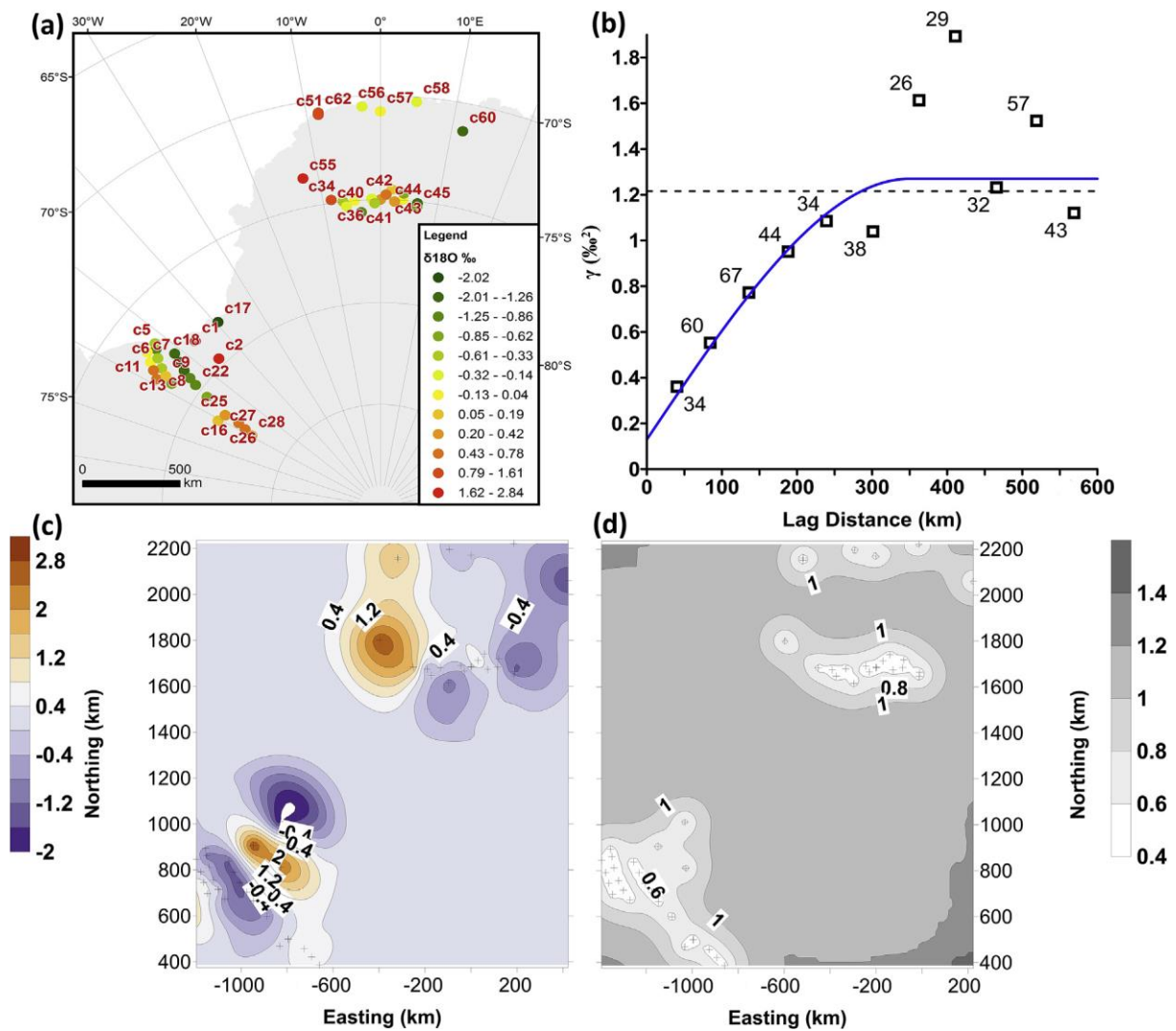


Fig. 4. Map of point residuals, variogram plot, and kriged map of the time average (1970-1988) $\delta^{18}\text{O}$ residuals and the standard deviation of kriging. (a) map of point residuals of the multiple regression; (b) empirical (blue squares) semivariogram and spherical theoretical model (blue line) ($C_0=0.13$; $C_0 + C=1.27$; $a=350$ km; $r^2=0.72$; bin width ~55 km) of the residuals. The variance is marked by the broken line. The numbers indicate the number of data pairs that were used to derive the variogram value (blue squares) for a particular bin in (b). (c) The ordinary point kriged map of the residuals; (d) the standard deviation of kriging. The faded crosses mark the locations of the ice cores in (c) & (d). Easting is the distance from the Prime Meridian, negative towards W and positive to E, while Northing is the distance from the South Pole, both in km.

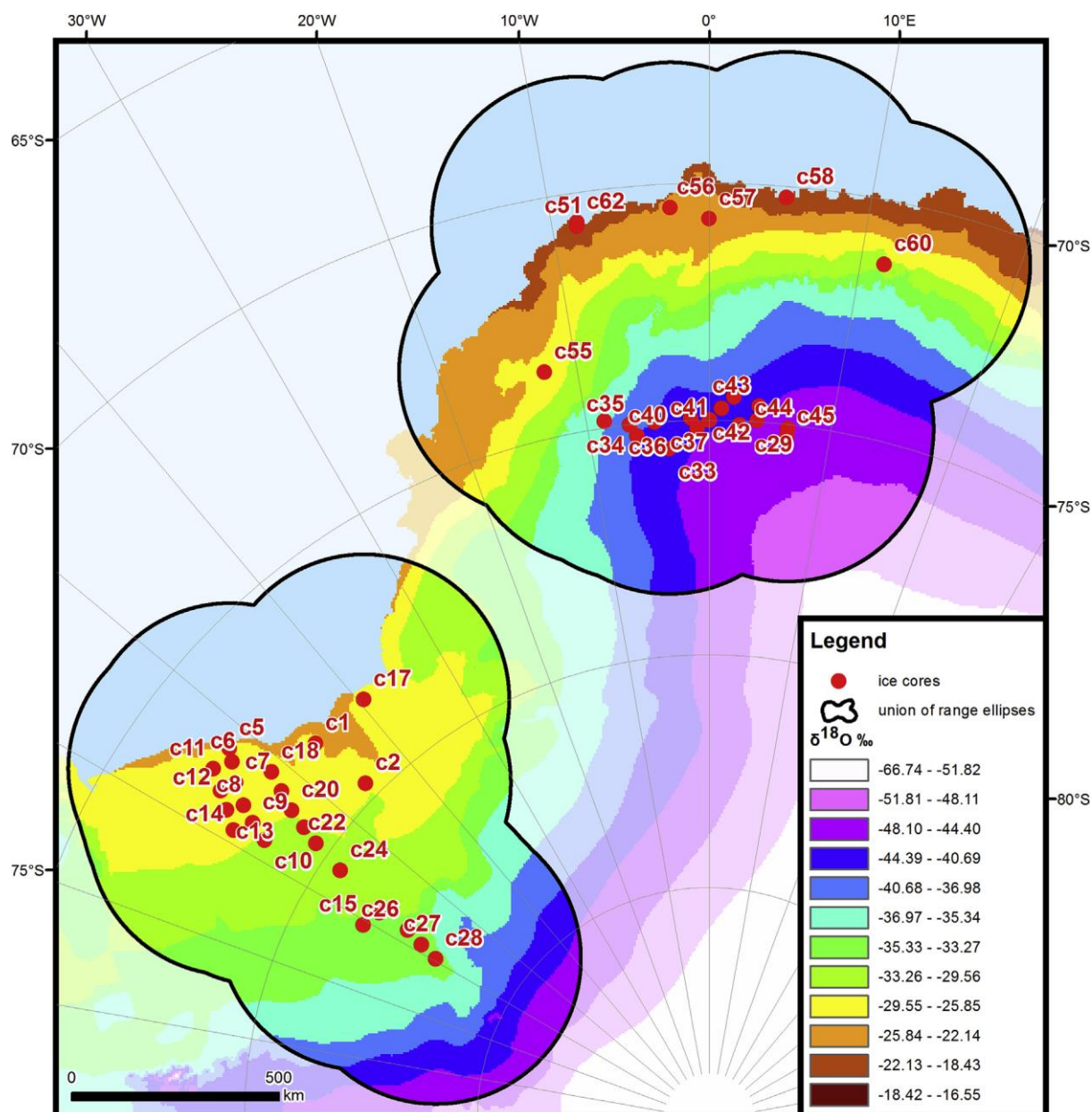


Fig. 5. Isoscape of $\delta^{18}\text{O}$ for the region for 1970-1988. The union of the 350km range ellipses is marked with a black line. Isotropy was assumed, as the direction subsets proved insufficient in the course of the exploration of anisotropy. Red dots mark the ice cores used in the study.

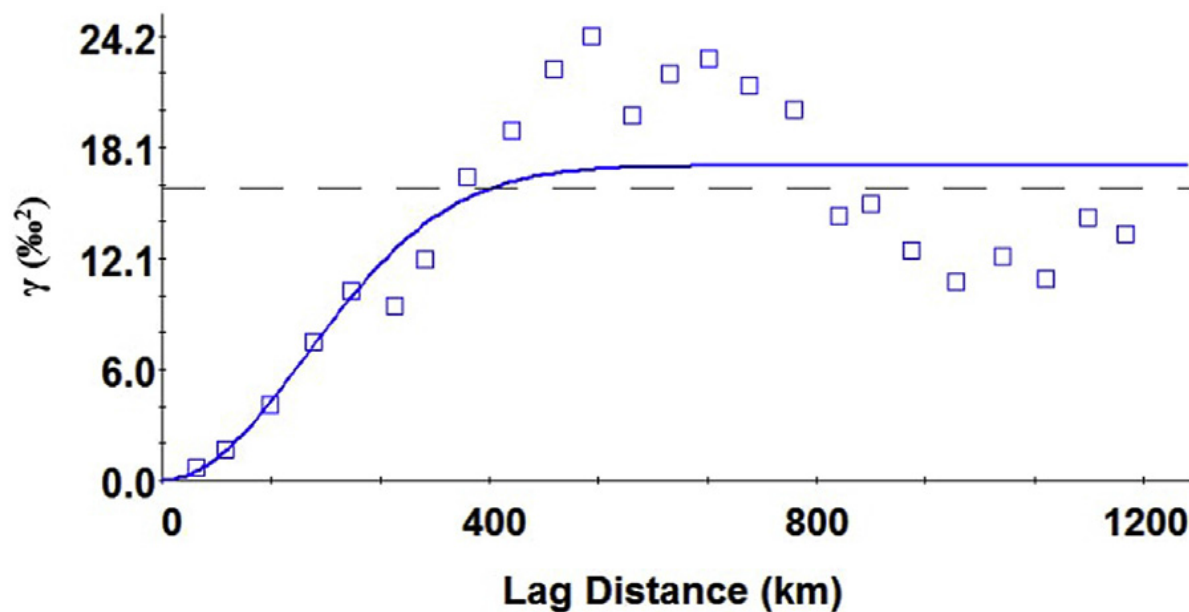


Fig. 6. Empirical semivariogram of residual near surface (2m) temperature data (see Table S3) for the region (1970-1988) marked with black squares and the fitted theoretical Gaussian model (blue line)

Tables

Table 1. Regression models of water stable isotopes using geographical variables in Antarctica overlapping with the study area

Study	Used independent variables	Estimated dependent variables	Scale
Masson-Delmotte et al., 2008	sin(LAT), ELE, D	$\delta^{18}\text{O}$, $\delta^2\text{H}$	Continental
Wang et al., 2010	LAT, LON, ELE, D	$\delta^{18}\text{O}$, $\delta^2\text{H}$	
Wang, 2009	$ \sin(\text{LAT}) ^2$, $ \sin(\text{LAT}) $, ELE	$\delta^{18}\text{O}$	
Altnau et al., 2015	ELE	$\delta^{18}\text{O}$	Regional
This study	LON, ELE, D	$\delta^{18}\text{O}$	