# **Response to editor comments**

Comments to the Author:

Dear Dr. Lavergne,

Thank you for submitting a revised version of your manuscript "Modelling tree-ring cellulose d18O variations of two temperature-sensitive tree species from North and South America". Please find a few additional minor suggestions and typos to correct. I also invite you to have another careful read of your manuscript, including figure legends and references.

Best regards,

Laurie Menviel

AC: We thanks the Editor for her additional suggestions in the text.

L. 44: "is more likely linked to the" do you want to say "is primarily linked to"?

AC: Yes. We have changed this part of the sentence as suggested by the Editor.

Move L. 133-134 (location of the model) to a new section "Code and data availability" to be added at the end of manuscript (right before the acknowledgment section.

Move L. 165-166 (IAEA web address) to the new section "Code and data availability"

Move L. 181-182: "extracted at http://paos.colorado.edu/~dcn/SWING/database.php" to the new section "Code and data availability"

Move L. 209: "provided by the NOAA/OAR/ESRL (https://www.esrl.noaa.gov/psd/data/gridded/data.20thC\_ReanV2c.html)," to the new section "Code and data availability"

Move L. 220: "http://cfs.nrcan.gc.ca/projects/3/4" to the new section "Code and data availability"

AC: We have added a 'Code and data availability' section before the Acknowledgement one as suggested by the Editor. We have moved in this new section all the references to each datasets used.

Please modify as follow:

L. 180: "1) The Melbourne University model (MUGCM)"

L. 183: "the Laboratoire de Météorologie Dynamique Zoom model (LMDZ5A)"

Please rephrase: L. 227 "as displayed in the observations" or "as shown"

L. 324: Please rephrase "are more highly correlated" as I don't think it is grammatically correct. Some suggestions: "are highly correlated" or "have a higher correlation coefficient"

Reviewer 1 suggested to use "tree rings" please use this spelling throughout the manuscript (i.e. change all the "tree-rings", e.g. title, section 2.1, legend of figure 1, keywords...).

L. 476: "we have provided"

L. 733: please add a space between "ones" and "with" or rephrase: "The tests sites from Quebec are in black and the Argentinean ones are in red."

Legend of figure 3: Please spell out "DOY"

AC: We have changed all the parts mentioned above as suggested by the Editor.

Legend of figure 4: "densities of probability of the coefficient of correlation" should it be instead "probability density functions"?

AC: We have changed 'densities of probability' into 'density distributions' in the legend of Figure 4, as done in Figure 5.

Figure 4 and 5: As already noted by Reviewer 1 the y axis should be "Kernel" and not "Kernal", please correct. Also in figure 5 the y axis should read "Kernel density estimate"

AC: We have corrected 'Kernal' into 'Kernel' in Figures 4 and 5, and the y axis legend of Figures 5 and SM3.

Modelling tree\_ring cellulose  $\delta^{18}$ O variations of two temperature-sensitive tree species from North and South America 2 3 4 **Authors:** 5 Aliénor Lavergne<sup>1</sup>, Fabio Gennaretti<sup>1</sup>, Camille Risi<sup>2</sup>, Valérie Daux<sup>3</sup>, Etienne Boucher<sup>4</sup>, Martine 6 M. Savard<sup>5</sup>, Maud Naulier<sup>6</sup>, Ricardo Villalba<sup>7</sup>, Christian Bégin<sup>5</sup> and Joël Guiot<sup>1</sup> 7 8 9 <sup>1</sup>Aix Marseille Université, CNRS, IRD, Collège de France, CEREGE, ECCOREV, Aix-en-10 Provence, France 11 <sup>2</sup>Laboratoirede Météorologie Dynamique, IPSL, UPMC, CNRS, Paris, France <sup>3</sup>Laboratoire des Sciences du Climat et de l'Environnement, CEA-CNRS-UVSQ, 91191 Gif-sur-12 13 Yvette, France 14 <sup>4</sup>Department of Geography and GEOTOP, Université du Québec à Montréal, Montréal, Canada <sup>5</sup>Geological Survey of Canada, Natural Resources Canada, 490 rue de la Couronne, QC, 15 16 G1K9A9, Canada 17 <sup>6</sup>Institut de Radioprotection et de Sureté Nucléaire (IRSN), PRP-ENV, SERIS/LRTE, Saint-Paullez-Durance, France 18 19 <sup>7</sup>Instituto Argentino de Nivología, Glaciología y Ciencias Ambientales, IANIGLA-CONICET, 20 Mendoza, Argentina 21 22 Corresponding authors: Aliénor Lavergne (alienor.lavergne@gmail.com) and Fabio Gennaretti 23 (gennaretti@cerege.fr) 24 Tel: +33 (0) 4 42 97 15 32

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#### ABSTRACT

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54 55 Oxygen isotopes in tree rings ( $\delta^{18}O_{TR}$ ) are widely used to reconstruct past climates. However, the complexity of climatic and biological processes controlling isotopic fractionation is not yet fully understood. Here, we use the MAIDENiso model to decipher the variability of  $\delta^{18}O_{TR}$  of two temperature-sensitive species of relevant paleoclimatological interest (Picea mariana and Nothofagus pumilio) and growing at cold high-latitudes in North and South America. In this first modelling study on δ<sup>18</sup>O<sub>TR</sub> values in both northeastern Canada (53.86°N) and western Argentina (41.10°S), we specifically aim at: 1) evaluating the predictive skill of MAIDENiso to simulate  $\delta^{18}O_{TR}$  values, 2) identifying the physical processes controlling  $\delta^{18}O_{TR}$  by mechanistic modelling and, 3) defining the origin of the temperature signal recorded in the two species. Although the linear regression models used here to predict daily  $\delta^{18}O$  of precipitation ( $\delta^{18}O_P$ ) may need to be improved in the future, the resulting daily  $\delta^{18}O_P$  values adequately reproduce observed (from weather stations) and simulated (by global circulation model)  $\delta^{18}O_P$  series. The  $\delta^{18}O_{TR}$  values of the two species are correctly simulated using the  $\delta^{18}O_P$  estimation as MAIDENiso input, although some offset in mean  $\delta^{18}O_{TR}$  levels is observed for the South American site. For both species, the variability of  $\delta^{18}O_{TR}$  series is primarily linked to the effect of temperature on isotopic enrichment of the leaf water. We show that MAIDENiso is a powerful tool for investigating isotopic fractionation processes but that the lack of a denser isotope-enabled monitoring network recording oxygen fractionation in the soil-vegetation-atmosphere compartments limits our capacity to decipher the processes at play. This study proves that the eco-physiological modelling of  $\delta^{18}O_{TR}$  values is necessary to interpret the recorded climate signal more reliably.

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**Supprimé:** rather than on the isotopic composition of the source water.

**Keywords:** MAIDENiso model,  $\delta^{18}$ O, tree ring, *Nothofagus pumilio*, *Picea mariana* 

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#### 1. INTRODUCTION

Oxygen isotopes in tree rings ( $\delta^{18}O_{TR}$ ) are increasingly used as indicators of past climatic 61 62 changes in temperate areas (Cernusak and English, 2015; Hartl-Meier et al., 2014; Saurer et al., 63 2008). They have been widely used to reconstruct past atmospheric conditions such as air 64 temperature (Naulier et al., 2015), drought (Labuhn et al., 2016), precipitation amount (Rinne et 65 al., 2013), isotopic composition of precipitation (Danis et al., 2006), relative air humidity 66 (Wernicke et al., 2015), cloud cover (Shi et al., 2012), and even atmospheric circulation patterns 67 (Brienen et al., 2012). This diversity of climatic targets possibly reconstructed based on oxygen 68 isotopes hints at the challenge of understanding the complexity of the climatic and biological processes that control isotopic fractionation of oxygen in trees (Treydte et al., 2014). 69 Uncertainties arise because different poorly measured factors influence  $\delta^{18}O_{TR}$  values. Isotopic 70 signals in tree rings cellulose are strongly influenced by isotopic signature of soil water taken up 71 72 by the roots and by evaporative and physiological processes occurring at the leaf level and during downstream metabolism (Barbour et al., 2005; Gessler et al., 2014). Thus, a comprehensive 73 74 approach that embraces existing mechanistic understanding of the fractionation processes 75 involved is required.

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Few isotopic process-based models have been developed to investigate the mechanistic rules governing the  $\delta^{18}O_{TR}$  variations (Guiot et al., 2014): the Péclet-modified Craig-Gordon model (Kahmen et al., 2011) and the Roden's model (Roden et al., 2000) are able to estimate, at a daily time step, the  $\delta^{18}O$  values of soil and xylem waters, and the isotopic fractionation occurring in the leaves due to evapotranspiration. Versions of these models are integrated in more complete forest ecophysiological models simulating the ensemble of forest water and carbon fluxes: (1) MAIDEN (Modeling and Analysis In DENdroecology) (Gea-Izquierdo et al., 2015; Misson, 2004), which contains the isotopic module MAIDENiso (Danis et al., 2012) and (2) MUSICA (Ogée et al., 2003, 2009). Both are accounting for important post-photosynthetic factors and are able to link photosynthesis and carbohydrate allocation to stem growth.

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In this paper, we use the MAIDENiso model to decipher the  $\delta^{18}O_{TR}$  variability in American temperature-sensitive species (*Picea mariana* in northeastern Canada and *Nothofagus pumilio* in western Argentina). The selected sites are of special interest for paleoclimatology given that their

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92  $\delta^{18}O_{TR}$  chronologies carry strong temperature signals. A summer temperature reconstruction was already developed at the North American site (Gennaretti et al., 2017b; Naulier et al., 2015) and a 93 calibration study conducted at the South American one highlighted the strong potential of  $\delta^{18}O_{TR}$ 94 95 values to reflect variations in summer-autumn temperatures over a large region south of 38°S (Lavergne et al., 2016). However, up to now, the climate- $\delta^{18}O_{TR}$  relationships were analysed 96 using a black box approach based on linear models. Here, we specifically aim at: 1) evaluating 97 98 the predictive skill of MAIDENiso to simulate  $\delta^{18}O_{TR}$  values, 2) identifying the physical processes controlling  $\delta^{18}O_{TR}$  by mechanistic modelling and, 3) defining the origin of the 99 100 temperature signal recorded in the two species.

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#### 2. DATA AND METHODS

#### 2.1. Sampling sites and tree-ring data

104 Two high-latitude American native species were studied here: 1) Picea mariana (Mill. B.S.P.; 105 black spruce), which is a conifer widely distributed over the American boreal forest (Viereck and 106 Johnston, 1990); and 2) Nothofagus pumilio (Poepp. et Endl. Krasser; lenga), which is an 107 angiosperm deciduous species dominating the high-elevation forests along the Patagonian Andes 108 from 35°S to 55°S (Donoso, 1981; Schlatter, 1994). We selected two sites of P. mariana in the 109 centre of the Quebec-Labrador Peninsula in northeastern Canada (L01 and L20; from 53°51'N-72°24'W to 54°33'N-71°14'W, ~480 m elevation; see Gennaretti et al. (2014) and Naulier et al. 110 111 (2014) for details) and three sites of N. pumilio in northern Patagonia, western Argentina (NUB, 112 ALM and CHA; from 41°09'S-71°48'W to 41°15'S-71°17'W, 1270-1610 m elevation; see 113 Lavergne et al. (2016, 2017) for details). Climate in northeastern Canada is mostly continental 114 and subarctic with short, mild and wet summers and long, cold and dry winter. Total annual 115 precipitation averages 825 mm with up to 46% falling during the growing season in summer 116 (June to September) (Naulier et al., 2014). In western Argentina, precipitation is largely 117 concentrated from late fall to early spring (May-November) followed by a drier and mild period 118 during summer and early fall (December-April) (López Bernal et al., 2012).

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Four trees per site were collected for both species. The selection of the samples and analytical procedure for  $\delta^{18}O_{TR}$  measurements were described in Lavergne et al. (2016) and Naulier et al.

(2014). The developed  $\delta^{18}O_{TR}$  chronologies covered the 1950-2005 and 1952-2011 periods at the northeastern Canadian and western Argentinian sites, respectively. The chronologies that were built for each species were significantly correlated between stands (Figure 1). This supported the construction of a combined isotope chronology for both the northeastern Canada and western Argentina sites.

### 2.2. Modelling oxygen isotopes in tree ring cellulose with MAIDENiso

MAIDENiso is a process-based model that can simulate in parallel phenological and meteorological controls on photosynthetic activity and carbon allocation (Danis et al., 2012). It explicitly allocates carbohydrates to different carbon pools (leaves, stem, storage and roots) on a daily basis using phenological stage-dependent rules (see Gennaretti et al. (2017b) for details on the construction of the main MAIDEN model). It also simulates the fractionation of carbon and oxygen isotopes during growth processes. In particular, it estimates at a daily time step  $\delta^{18}$ O values of soil water and xylem water, the isotopic fractionation occurring in the leaves due to evapotranspiration and the biochemical fractionation during cellulose formation. It uses as input daily maximum and minimum temperature (°C), precipitation (cm/day), atmospheric CO<sub>2</sub> concentration (ppm) and  $\delta^{18}$ O values of precipitation ( $\delta^{18}$ O<sub>P</sub> in %).

In this study, the calculation of the daily  $\delta^{18}O_{TR}$  in tree ring cellulose (‰) is based on the (Danis et al., 2012)'s formulation of the Craig-Gordon model (Craig and Gordon, 1965):

$$\delta^{18}O_{TR} = (1 - f_o) \cdot [\epsilon^* + \epsilon_k \cdot (1 - h_{air}) + h_{air} \cdot \delta^{18}O_V + (1 - h_{air}) \cdot \delta^{18}O_{XW}] + f_o \cdot \delta^{18}O_{XW} + \epsilon_0$$
 (1)

This equation summarizes how  $\delta^{18}O_{TR}$  is determined by:

- (i) the  $\delta^{18}O$  of the source (xylem) water ( $\delta^{18}O_{XW}$ ), which is computed by averaging the  $\delta^{18}O_{SW}$  values of the different soil layers weighted by the volume of water taken up by the roots in each layer. The isotopic effects of water mixing and soil evaporation on the  $\delta^{18}O_{SW}$  values of the different soil layers are computed by a mass and isotopic balance (Danis et al., 2012). It is worth noting that no fractionation occurs during water uptake by roots (Wershaw et al., 1966), neither during the transport of water from the roots to the leaves.
- (ii) the <sup>18</sup>O enrichment of the leaf water due to transpiration is described by  $(\epsilon^* + \epsilon_k \cdot (1 h_{air}) + h_{air} \cdot \delta^{18} O_V + (1 h_{air}) \cdot \delta^{18} O_{XW})$  after Craig and Gordon (1965), where:

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a. ε\* is the equilibrium fractionation due to the change of phase from liquid water to vapour at the leaf temperature (fixed at 21.4°C, the temperature threshold for maximum carbon assimilation, ε\* is 9.65% (Helliker and Richter, 2008)),

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- b.  $\varepsilon_k$  is the kinetic fractionation due to the diffusion of vapour into unsaturated air through the stomata and the leaf boundary layer,
- c. h<sub>air</sub> is the relative humidity of the evaporating air mass estimated from daily air temperature (T<sub>air</sub>; °C; mean of the maximum and minimum air temperatures), and the dew point temperature (T<sub>r</sub>; °C) (Running et al., 1987),
- d.  $\delta^{18}O_V$  is the atmospheric water vapour calculated assuming a precipitation-vapour isotopic equilibrium (see below);
- (iii) the biochemical fractionations ( $\epsilon_0$ ) due to oxygen exchange between carbonyl groups (C = O) in the organic molecules and water (DeNiro and Epstein, 1979; Farquhar et al., 1998).
- (iv) the dampening factor  $f_o$  reflecting the exchange of the oxygen atoms between sucrose and xylem water during cellulose synthesis in the xylem cells of tree rings.
- 175 As previously evoked (i),  $\delta^{18}O_{XW}$  of Eq. 1 depends on  $\delta^{18}O_{SW}$  and thus on  $\delta^{18}O_P$  values. However, 176 long continuous time series of  $\delta^{18}O_P$  are not available in the studied area. Here, we tested the 177 impact of using two different methods for deriving  $\delta^{18}O_P$  time series.
- First, a linear model was used to estimate the daily values of  $\delta^{18}O_P$  and subsequently  $\delta^{18}O_V$  based on the primary drivers of their temporal variability (Dansgaard, 1964; Horita and Wesolowski,
- 180 1994), that are air temperature ( $T_{air}$ ; °C) and precipitation at the corresponding site (P; mm):

$$\delta^{18}O_{P} = a \cdot T_{air} + b \cdot P + c \tag{2}$$

$$\delta^{18}O_V = \delta^{18}O_{P} - \epsilon^*_{Tair}$$
 (3)

- with  $\varepsilon^*_{Tair}$  the fractionation due to the change of phase from liquid water to vapour at the mean air temperature. The coefficients a and b were allowed to vary over a plausible range (or prior range) in the calibration process together with other MAIDENiso parameters, while coefficient c was fixed to a likely value (see Table 1 and section 2.4). This estimated set of data is referred in the following as the estimated  $\delta^{18}O_P$  dataset.
- Second, we run the model with the series of the daily  $\delta^{18}O_P$  derived from two general circulation models (GCM) with different spatial resolutions and enough available data at our site locations:

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1) the Melbourne University model (MUGCM; Noone and Simmonds, 2002) forced by varying sea surface temperature (SST) from the HadISST data set for the 1950-2003 period ( $2^{\circ}\times2^{\circ}$  resolution; hereafter referred as MUGCM  $\delta^{18}O_P$  dataset), and 2) the Laboratoire de Météorologie Dynamique Zoom model (LMDZ5A; Hourdin et al. (2013); Risi et al. (2010)) with the horizontal winds guided by those of the National Centers for Environmental Protection -  $20^{th}$  Century Reanalysis (NCEP20) for the 1950-2008 period (Compo et al., 2011) ( $2.5^{\circ}\times3.75^{\circ}$  resolution; hereafter referred as LMDZ-NCEP20  $\delta^{18}O_P$  dataset).

The final  $\delta^{18}O_{TR}$  time series are the annual average of the  $\delta^{18}O_{TR}$  daily values (Eq. 1) weighted by the daily simulated stand Gross Primary Production (GPP), assuming a proportional allocation of carbon to the trunk. For the northeastern Canadian sites, the GPP simulated by MAIDENiso was optimized using observations from an eddy covariance station (see Gennaretti et al. (2017a)). Unfortunately, such observations were not available for N. pumilio, and therefore the parameterization obtained for the GPP of P. mariana was also used for the western Argentinian sites but constraining the simulations with phenological observations extracted from the literature. For example, to respect the annual cycle of the leaf area index (LAI) for N. pumilio (Magnin et al., 2014; Rusch, 1993), we used in MAIDENiso a seasonal LAI annual cycle with a development of leaves (LAI increase) between October and November, a maximum LAI (set at 5 leaf area/ground area) from November to April, a decreasing LAI (leaf fall) between April and May, and finally a leafless period (null LAI) from June to September (Magnin et al., 2014; Rusch, 1993). Furthermore, based on the finding that  $\delta^{18}O_{TR}$  annual time series were more correlated to climate variables of specific months of the growing season (Lavergne et al., 2016), we also computed  $\delta^{18}O_{TR}$  annual values by weighting the  $\delta^{18}O_{TR}$  daily values (Eq. 1) with synthetic GPP time series maximizing the correspondence between observations and simulations.

# 2.3. Meteorological and atmospheric CO<sub>2</sub> data

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At the western Argentinian sites, we did not have long daily records of observed climate data. Therefore, daily minimum–maximum temperature and precipitation data were derived from the 20th Century Reanalysis V2c (2°×2° resolution; Compo et al., 2011), which is one of the few reanalysis products covering entirely the 20th century. The temperature daily time series of the reanalysis were corrected in order to respect the monthly mean values detected at Bariloche, the

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https://www.esrl.noaa.gov/psd/data/gridded/data.20t hC ReanV2c.html), 238 nearest meteorological station from our sampling sites (~48 km from the sites, 41°12′ S-71°12′ 239 W, 840 m asl; Servicio Meteorológico Nacional, Argentina). The resulting maximum and minimum temperature series, covering the 1952-2011 period, fit well with the daily local 240 241 temperature data from La Almohadilla (ALM) site (41°11'S, 71°47'W, 1410 m asl; data 242 measured by dataloggers and provided by IANIGLA) available over the 2002-2012 period (r = 243 0.74, p < 0.001; Figure SM1). For the northeastern Canadian sites, climate data were obtained 244 from the gridded interpolated Canadian database of daily minimum-maximum temperature and precipitation covering the 1950-2005 studied period (0.08°×0.08° resolution. Hutchinson et al., 245 246 2009). In addition to these data we also used modelled daily data from the GCMs described 247 above for both the western Argentinian and northeastern Canadian sites (see Table 2 with the input data used for each tested configuration). 248

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Data on the atmospheric  $CO_2$  concentration were derived from the Mauna Loa station over the 1958-2012 period (Keeling et al., 1976). For the years 1950-1957, we extrapolated atmospheric  $CO_2$  data using the trend and seasonal cycle as displayed in the observations over the subsequent 10-years period (1958-1967).

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# 2.4. Estimation of parameters influencing $\delta^{18}O_{TR}$

We used a Bayesian method for the simultaneous calibration of the various MAIDENiso parameters specific to the study species and site. A set of 50 plausible blocks of parameters (posterior values) was selected according to the method described in Gennaretti et al. (2017a) using Markov Chain Monte Carlo (MCMC) sampling (Table 1). The following prior plausible ranges were considered:

1) the prior ranges of the a and b coefficients in the equation of the daily  $\delta^{18}O_P$  (Eq. 2) were selected in order to get  $\delta^{18}O_P$  values for each site consistent with the measured monthly local values from the nearest stations of the Global Network of Isotopes in Precipitation (GNIP), and with the simulated daily values from the LMDZ-NCEP20 model and from the MUGCM model

(see Table 1),
266 2) the range for the biochemical fractionation factor ε<sub>0</sub> was chosen between 24% and 30%

(+27±3% after DeNiro and Epstein (1981), Sternberg (1989) and Yakir and DeNiro (1990)),

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3) the range for the kinetic fractionation  $\varepsilon_k$ , which has been set to 26.5% in Farquhar et al. (1989) but that can vary over larger ranges (Buhay et al., 1996), was taken between 10% and 30% here,

4) the range for the dampening factor  $f_o$  was allowed to vary between 0.3 and 0.5 following

280 Saurer et al. (1997).

We tested the sensitivity of the MAIDENiso model to the calibrated parameters by modifying them within their respective prior calibration range. To control the robustness of the calibrated parameters, we performed the calibration of these parameters over two equal length intervals (1950-1977 and 1978-2005 for *P. mariana*; 1952-1981 and 1982-2011 for *N. pumilio*) keeping the second half for independent validation of the parameters estimates. Once the model was calibrated for the two species, the MAIDENiso's performance to simulate *P. mariana* and *N. pumilio*  $\delta^{18}O_{TR}$  interannual data was evaluated using the correlation coefficients (r) and the root mean square errors (RMSE) between observed and simulated values. This is a standard approach to evaluate how well a mechanistic model is simulating  $\delta^{18}O_{TR}$  variations (e.g., Danis et al., 2012; Lorrey et al., 2016).

# 2.5. Disentangling leaf-level fractionation processes and source water influences on $\delta^{18}O_{TR}$ signature

To define the relative contributions to the  $\delta^{18}O_{TR}$  signature of the isotopic signal of the source water (xylem water) and of the fractionation processes due to transpiration taking place in the leaves, we designed two experimental simulations with MAIDENiso based on Eq. 1:

- 1) to quantify the influence of the variability of the isotopic composition of the xylem water on  $\delta^{18}O_{TR}$ , we compared the reference simulations to those where the relative humidity (h<sub>air</sub>) and the isotopic composition of atmospheric vapour ( $\delta^{18}O_V$ ) were assumed to be constant. The constant values for h<sub>air</sub> and  $\delta^{18}O_V$  were defined as the averages of the respective MAIDENiso outputs (h<sub>air</sub> = 0.62 and 0.9, and,  $\delta^{18}O_V$  = -26.28% and -17.34%, respectively for northeastern Canada and western Argentina; the XW source experiment simulation hereafter),
- 2) to quantify the influence of the isotopic enrichment of the leaf water due to transpiration on  $\delta^{18}O_{TR}$ , we compared the reference simulations to those where the  $\delta^{18}O_{XW}$  series were assumed to be constant. The constant value for  $\delta^{18}O_{XW}$  was estimated as the average of

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the  $\delta^{18}O_{XW}$  MAIDENiso outputs ( $\delta^{18}O_{XW}$  = -13.81% and -7.03%, respectively for northeastern Canada and western Argentina; the Leaf water enrichment driven experiment simulation hereafter).

Comparison between the experimental and reference simulations (i.e. using the optimal values of the parameters) was achieved through the calculation of the coefficient of determination  $(R^2)$ .

#### 3. RESULTS

# 3.1. Estimated versus modelled and observed δ<sup>18</sup>O<sub>P</sub> values

The modelled  $\delta^{18}O_P$  series from the GCM models are similar to the GNIP datasets, with mean values ranging from -12‰ to -8‰ over June-September in northeastern Canada (Figure SM2A) and from -7‰ to -3‰ over December-April at the western Argentinian sites (Figure SM2B). In general,  $\delta^{18}O_P$  series from LMDZ-NCEP20 model in western Argentina are slightly displaced toward higher values (+1‰) in comparison with the GNIP and MUGCM data. The estimated  $\delta^{18}O_P$  values based on plausible values of coefficients a and b agree well with those of the models and observations in northeastern Canada. For the western Argentinian sites, they are 2-3‰ lower from April to October, i.e. late spring-early autumn (Figure SM2).

#### 3.2. Sensitivity of the model to the calibrated parameters

Most of the calibrated parameters have an influence on the correlations between observed and simulated  $\delta^{18}O_{TR}$  series and/or on the mean levels of the simulated series (Figure 2). The temperature and precipitation dependences of  $\delta^{18}O_P$  values (respectively a and b coefficients) have the strongest influence on correlations. Increasing a and b values increase the mean  $\delta^{18}O_{TR}$  levels, more strongly in western Argentina than in northeastern Canada (Figure 2). Changes in the dampening factor ( $f_o$ ) and in the biochemical fractionation ( $\epsilon_0$ ) have almost no effect on correlation, but their increase induces significant decrease of the mean levels of  $\delta^{18}O_{TR}$  series. Finally, increasing the kinetic fractionation ( $\epsilon_k$ ) leads to lower correlations and to higher mean levels of  $\delta^{18}O_{TR}$  (Figure 2).

# 3.3. MAIDENiso performance in reproducing observed $\delta^{18}O_{TR}$ series

Split-period verifications of the calibrated relationships for *P. mariana* and *N. pumilio* when using estimated  $\delta^{18}$ O<sub>P</sub> series from Eq. 2 indicate that the calibration over either the first half or the

second half periods provide similar posterior densities of the calibrated parameters than the ones obtained when calibrating over the whole periods (Figure SM3). One exception is observed in the calibration of coefficient a in northeastern Canada over the two half periods, where the posterior densities of a are different from the one obtained by calibrating over the entire period. Over the entire periods, observed and simulated  $\delta^{18}O_{TR}$  series are significantly correlated in northeastern Canada (r = 0.56, p < 0.01 and RMSE = 0.67; Figure 3A) and in western Argentina (r = 0.48, p < 0.01 and RMSE = 0.63; Figure 3C). The correlation between observed and simulated  $\delta^{18}O_{TR}$ series are slightly improved when we used synthetic daily GPP (r = 0.62 and r = 0.52, p < 0.01. respectively for northeastern Canada and western Argentina; Figure 3B and 3D). It is worth noting that the mean levels of the simulated  $\delta^{18}O_{TR}$  series for the Argentinian sites are lower than those of the observations (offset of around -2.5%; Figure SM4). The series were therefore corrected to respect the mean values detected in the observations (Figure 3C and 3D). In contrast, the correlations between observation and simulation considerably decrease when we used modelled δ<sup>18</sup>O<sub>P</sub> from MUGCM models or LMDZ-NCEP20 reanalysis data. They only reach r = 0.13 (p > 0.05) to 0.23 (p < 0.05) in northeastern Canada and r = 0.23 to 0.26 (p < 0.05) in western Argentina, respectively (Figure 4).

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# 3.4. Influence of source water and leaf water isotopic enrichment to the $\delta^{18}O_{TR}$ signature

The relative contributions to the  $\delta^{18}O_{TR}$  signature of the isotopic signal of the source (xylem) water and of the  $^{18}O$  enrichment of the leaf water due to transpiration were investigated. In both regions, the Leaf water enrichment experimental simulations and the reference simulations have a higher correlation coefficient ( $R^2$  centred on 0.9 and 0.95, respectively for northeastern Canada and western Argentina; Figure 5) than are the XW source simulations with the reference simulations ( $R^2$  centred on 0.65 and 0.8, respectively for northeastern Canada and western Argentina). This suggests that, with the model, the variability of  $\delta^{18}O_{XW}$  has a weaker influence on  $\delta^{18}O_{TR}$  variations than the changes of the leaf water isotopic enrichment do. Notably, *P. mariana* in northeastern Canada appears to be more sensitive to both influences than *N. pumilio* in western Argentina (Figure 5).

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# 4. DISCUSSION

# 4.1. Precipitation $\delta^{18}O_P$ variations and estimation

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Although the regression models used to predict daily δ<sup>18</sup>O<sub>P</sub> values are likely too simplistic, the resultant monthly averaged values adequately reproduce the distribution of the observed (from GNIP stations) and modelled (by GCMs) monthly  $\delta^{18}O_P$  series in northeastern Canada. In western Argentina, the distribution of monthly  $\delta^{18}O_P$  values is also well reproduced but the amplitude of variation of the predicted values is too high, leading to simulated values lower than the measured ones during the colder months. The temporal  $\delta^{18}$ O<sub>P</sub> variations are positively related to air temperature given the positive coefficient a. In agreement with the simple Rayleigh distillation model (Dansgaard, 1964), as air temperature decreases, the specific humidity at saturation decreases, and water vapour condenses. H<sub>2</sub><sup>18</sup>O condenses preferentially, the residual water vapour gets more and more depleted as condensation proceeds. Consequently, in the Tropics, the <sup>18</sup>O/<sup>16</sup>O ratio in the meteoric water has been observed to decrease with increasing amount of precipitation and/or relative humidity (Rozanski et al., 1993). In extra-tropical regions,  $\delta^{18}O_P$  may also correlate with precipitation amount (negative coefficient b), since both variables depend on the meteorological conditions. The results of the linear regressions show comparatively lower influence of precipitation on  $\delta^{18}O_P$  in western Argentina than in northeastern Canada (Table 1). This suggests that the imprint of the precipitation amount on  $\delta^{18}O_P$  in western Argentina is low and that  $\delta^{18}O_P$  variations are

The results of the linear regressions show comparatively lower influence of precipitation on  $\delta^{18}O_P$  in western Argentina than in northeastern Canada (Table 1). This suggests that the imprint of the precipitation amount on  $\delta^{18}O_P$  in western Argentina is low and that  $\delta^{18}O_P$  variations are mainly controlled by seasonal changes in temperature, which is in agreement with previous work (Rozanski et al., 1995). However, due to the strong west-to-east precipitation gradient in this region (orographic rain shadow), large  $\delta^{18}O_P$  variations occur over short distances (Rozanski et al., 1995; Smith and Evans, 2007; Stern and Blisniuk, 2002). Therefore, the daily precipitation dataset extracted from the gridded reanalysis data, which has a low spatial resolution (>200 km), may not represent the daily variations in precipitation at a local scale faithfully. Therefore, the model may underestimate the contribution of precipitation on  $\delta^{18}O_P$  variability in this particular area.

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In contrast, in northeast Canada, both temperature and precipitation amount equally control the  $\delta^{18}O_P$  variations. The high amount of precipitation falling in summer (~46%) should have a strong effect and decrease the  $\delta^{18}O_P$  values in the condensed water, while high temperatures counteract this effect by increasing this ratio. Before reaching northeastern Canada, the air masses pushed by the dominant westerly winds discharge most of their humidity over the land,

leading to a depleted  $\delta^{18}O_P$  signal at our sites (for the same reason,  $\delta^{18}O_{TR}$  values at L20, which is located 110 km North-East of L01, are ~1% lower). Moreover, the  $\delta^{18}O_P$  signal in the Canadian sites is comparatively more depleted than in the Argentinian sites, because of their higher latitude. It is worth noting that the resolution of the gridded meteorological dataset used for the Canadian sites is relatively high (~10 km), which means that the local processes are likely well represented.

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# 4.2. Relative performance in modelling $\delta^{18}O_{TR}$ values

The simulated  $\delta^{18}O_{TR}$  series based on daily  $\delta^{18}O_P$  estimation from the regression models reproduce the observations better than the ones based on  $\delta^{18}O_P$  values derived from GCMs (Figure 4). This is in part due to the greater number of parameters to optimize, as the calibration process can more easily find a solution that fits the observations better. This may however reflect error compensations especially in western Argentina where the estimated annual variability of  $\delta^{18}O_P$  is too large. Conversely in northeastern Canada, the annual variations of  $\delta^{18}O_P$  that are estimated, simulated by GCMs and observed are in good agreement (Figure SM2). Although isotope-enabled atmospheric global models can reproduce the mean annual precipitation isotopic values and seasonality for many areas (Risi et al., 2010), results at specific sites, especially in mountainous regions such as at our western Argentinian site, can be less accurate (Figure SM2; see the offset between GNIP stations and LMDZ-NCEP20). Ideally, daily δ<sup>18</sup>O<sub>P</sub> long-term records from meteorological stations in the study region should be used as an input of MAIDENiso. Simulations from high-resolution regional circulation models, such as REMOiso which has a 0.5°×0.5° (~55 km) horizontal resolution (Insel et al., 2013; Sturm et al., 2007, 2005), may produce reliable local  $\delta^{18}O_P$  values. Such dataset has proven to be quite helpful with MAIDENiso in the Fontainebleau forest (France) (Danis et al., 2012). However, up to now, measured or REMOiso  $\delta^{18}O_P$  datasets in our regions of study do not exist, which is the case for most regions of the world. Moreover, early data (1970-80s) from GNIP stations may have been compromised by pan evaporation and therefore isotopic enrichment. Therefore, we recommend that daily GNIP stations are set up in various forested ecosystems, that an effort is accomplished to homogenize older GNIP time series, and that high resolution simulations of  $\delta^{18}O_P$  are performed in wider regions.

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The modelling of  $\delta^{18}O_{TR}$  values based on the estimation of  $\delta^{18}O_{P}$  is relatively more accurate for 435 northeastern Canada than for western Argentina (Figure 3). As the mean levels of the measured 436  $\delta^{18}O_{TR}$  values are high at the western Argentinian sites (mean value of about 30%), the Bayesian 437 optimization tends to increase the biochemical  $(\varepsilon_0)$  and kinetic  $(\varepsilon_k)$  fractionations as well as the 438 439 coefficient a, while reducing the dampening factor  $(f_0)$  to reach more representative mean levels 440 of the  $\delta^{18}O_{TR}$  simulation. But still, these levels are too low in comparison with the observations 441 (about 2.5% lower; Figure SM4). When the posterior value of a calibrated parameter is limited to 442 the upper bound of the prior range of plausible values, as it is the case at the western Argentinian 443 sites for a, b and  $\varepsilon_0$  (Figure SM3), it means that either the prior range is too narrow, or the model 444 is inadequate, or some important process is not considered in the model. Here, the estimation of 445 the prior ranges of both coefficients a and b were based on observed (GNIP stations) and simulated (GCMs)  $\delta^{18}O_P$  values. Therefore, we expect their respective ranges to be consistent 446 447 with local processes. When the prior range of a is extended to higher values in the optimization 448 process, observed and simulated  $\delta^{18}O_{TR}$  mean levels in western Argentina are better matching. However, in this case, the distribution of  $\delta^{18}O_P$  values is shifted toward higher values, advocating 449 450 for unrealistic estimated  $\delta^{18}O_P$  variations. 451 One other possibility is that the prior range of  $\varepsilon_0$  is too narrow. In accordance with DeNiro and 452 Epstein (1981), Sternberg (1989) and Yakir and DeNiro (1990), the biochemical fractionation  $\varepsilon_0$ 453 is assumed here to be lower than 30%. However, a recent study has demonstrated that this 454 parameter, nearly constant between 20 to 30°C, increases at lower temperatures to values of 31% 455 (Sternberg and Ellsworth, 2011). During the growing season, maximum temperatures can reach 456 20°C in western Argentina and 30°C in northeastern Canada, which suggests that the high mean δ<sup>18</sup>O<sub>TR</sub> levels in N. pumilio may be due to biochemical fractionation higher than 30% due to 457 temperature generally lower than 20°C. However, when the prior range of  $\varepsilon_0$  is extended to 31% 458 in the optimization process, the mean  $\delta^{18}O_{TR}$  levels of N. pumilio are still too low in comparison 459 460 with the observations. These results advocate for the existence of other processes, which can explain this offset in mean levels in Argentina. For example, higher soil water evaporation than 461 modelled by MAIDENiso should lead to less negative  $\delta^{18}O_{SW}$  (and therefore  $\delta^{18}O_{XW}$ ), which 462 could explain the high mean levels of  $\delta^{18}O_{TR}$  in Argentina. Caution should be exercised with such 463 an interpretation since other species living in similar conditions as N. pumilio in western 464 Argentina show comparatively lower mean  $\delta^{18}O_{TR}$  levels than N. pumilio (i.e., Fitzroya 465

cupressoides; see Lavergne et al., 2016). The ongoing monitoring and evaluation of isotopic processes based on synchronous measurements of vapour, precipitation, soil water and xylem water will certainly help understanding the high mean levels observed in Argentina, and increasing the representation of the involved processes in MAIDENiso.

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The better fit between observed and simulated  $\delta^{18}O_{TR}$  values obtained with specific forms of synthetic distributions of daily GPP for northeastern Canada and western Argentina (Figure 3) suggests differential limiting factors in the two regions. The synthetic bimodal distribution of daily GPP with maxima in spring and autumn, as simulated in western Argentina, is often observed in a diversity of ecosystems such as in the Mediterranean environments (Baldocchi et al., 2010; Gea-Izquierdo et al., 2015). After the activation of the photosynthesis in early spring, increasing temperatures tend to be optimal for tree growth. However, in a modelling study, Lavergne et al. (2015) have shown that the influence of temperature on N. pumilio's growth becomes negative once a temperature threshold (soil moisture) is exceeded. Therefore, we assume that after reaching a threshold of temperature and soil moisture summer conditions, tree growth is inhibited, leading to a decrease of primary productivity. However, when temperature starts to decline and soil water supply tends to increase with increasing precipitation events, tree growth increases again until the end of the growing season. In contrast, because precipitation is more abundant in summer (June to September) in northeastern Canada (Naulier et al., 2014), high summer temperatures should be always beneficial to tree growth if enough soil water is available. Therefore, in agreement with GPP-derived eddy covariance data from the Fluxnet network (see Gennaretti et al., 2017a), a better fit between observations and simulations is observed when using a unimodal rather than a bimodal GPP distribution. Monitoring of tree physiology, environmental conditions and wood cell formation will provide a more detailed representation of the complex biological and ecological processes operating in Patagonia, allowing us to run the MAIDENiso model with better constraints.

# 4.3. What is the main origin of the temperature signal recorded in $\delta^{18}O_{TR}$ ?

The investigation of the relative contributions of the isotopic composition of the source (xylem) water and of the  $^{18}$ O enrichment of the leaf water by transpiration on the simulated  $\delta^{18}$ O<sub>TR</sub> reveals that the variability of the former has a weaker influence on  $\delta^{18}$ O<sub>TR</sub> variations than that of the

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latter in North and South America. Therefore, the temperature signal recorded in  $\delta^{18}O_{TR}$  series more likely reflects the effect of temperature on isotopic enrichment of the leaf water rather than on the isotopic composition of the source water. At the leaf-level, air temperature has a strong effect on the relative humidity and therefore on the vapour pressure deficit (VPD), i.e. the difference between the saturation vapour pressure and the actual vapour pressure, which modulates the transpiration (Barbour, 2007). Thus, the imprint of the ambient air temperature on the fractionation processes occurring during transpiration is preferentially recorded in the tree rings of the two species. Furthermore, both the isotopic signature of the xylem water and of the fractionation processes occurring at the evaporation sites of the leaves have comparatively higher influence on  $\delta^{18}O_{TR}$  in P. mariana than in N. pumilio. This is probably due to the lower amplitude of the day-by-day variations of the relative humidity in western Argentina (SD = 5%) versus in northeastern Canada (SD = 16%) that translates into a weaker influence of hair variations and therefore of leaf-level isotopic fractionation processes on  $\delta^{18}O_{TR}$  values in western Argentina than in northeastern Canada. These results highlight the potential of MAIDENiso model to better refine the origin of the climatic signal recorded in the oxygen isotopic signature in the tree rings of different species.

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#### 5. CONCLUSION

Here, by using MAIDENiso model, we have provided a mechanistic overview of the climatic and biological processes controlling oxygen isotopic fractionation in two American temperature-sensitive tree species. First, we have shown that using regression-based rather than model-based  $\delta^{18}O_P$  estimates as inputs increases the predictive skills of our simulations, although this may be at the price of error compensations. Second, our study reveals that the variability of the isotopic composition of the source (xylem) water has a weaker influence on  $\delta^{18}O_{TR}$  variations than that of the  $^{18}O$  enrichment of the leaf water by transpiration. Last, these findings suggest that the imprint of temperature recorded in  $\delta^{18}O_{TR}$  of the two species is likely related to the effect of temperature on isotopic enrichment of the leaf water. The isotopic monitoring of water within the soil-vegetation-atmosphere compartments in future work will certainly provide the input and control data necessary to better constrain MAIDENiso. Our study demonstrates that the ecophysiological modelling of  $\delta^{18}O_{TR}$  values is necessary and likely the only approach to accurately interpret the recorded climate signal. Based on the calibrations of MAIDENiso presented here,

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534 the next step involves inverse modelling approaches to perform paleoclimatic reconstructions in 535 North and South America that are less biased by the complex and nonlinear interactions between 536 climate, CO<sub>2</sub> concentrations and tree growth as recommended by Boucher et al. (2014). 537 538 Code and data availability The code of the model can be found in https://doi.org/10.6084/m9.figshare.5446435.v1. The daily 539 540  $\delta^{18}O_P$  data from the MUGCM model were extracted via the SWING project webpage (http://paos.colorado.edu/~dcn/SWING/database.php). The daily climatic data used for Quebec 541 542 were retrieved from http://cfs.nrcan.gc.ca/projects/3/4, while those for Argentina were extracted 543 from https://www.esrl.noaa.gov/psd/data/gridded/data.20thC ReanV2c.html. The atmospheric CO<sub>2</sub> concentration data derived from the Mauna Loa station were extracted from 544 545 http://www.esrl.noaa.gov/gmd/ccgg/trends/. 546 547 **ACKNOWLEDGMENTS** 548 A.L. has been supported by a Research associate/Lecturer position at the Aix-Marseille 549 University (France). F.G. has received funding from the European Union's Horizon 2020 550 research and innovation program under the Marie Sklodowska-Curie grant agreement No 551 656896. We acknowledge all data providers: the Instituto Argentino de Nivología, Glaciología y 552 Ciencias Ambientales (IANIGLA, Argentina) for providing the daily temperature data from La 553 Almohadilla site; the National Meteorological Service from Argentina for providing the monthly temperature data from Bariloche meteorological station (Argentina); the Department of Natural 554 555 Resources Canada for providing the daily climatic data used for Quebec; the US Department of 556 Energy, Office of Science Biological and Environmental Research (BER) and the National Oceanic and Atmospheric Administration Climate Program Office for providing the daily 557 climatic data used for Argentina; and the SWING project for providing the daily  $\delta^{18}O_P$  data from 558

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# **Tables and Figures**

**Table 1** Definition of sensitive parameters. The posterior medians and 90% confidence intervals are also shown.

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Parameter	Definition	Unit	Parameter type (prior range)	Values with 90% posterior confidence intervals
$f_o$	Dampening factor	NA	Calibrated (0.3 to 0.5)	0.36 [0.31; 0.46] (Arg.) 0.41 [0.32; 0.48] (Q.)
$\epsilon_0$	Biochemical fractionation	%00	Calibrated (24 to 30)	29.99 [29.93; 30] (Arg.) 26.81 [24.74; 28.04] (Q.)
$\epsilon_k$	Kinetic fractionation	<b>%</b> o	Calibrated (10 to 30)	28.86 [18.25; 29.96] (Arg.) 17.20 [11.16; 26.34] (Q.)
а	Temperature dependence of $\delta^{18}O_P$	NA	Calibrated (0.2 to 0.5 for Arg. and 0 to 0.38 for Q.)	0.50 [0.49; 0.50] (Arg.) 0.31 [0.25; 0.37] (Q.)
b	Precipitation dependence of δ <sup>18</sup> O <sub>P</sub>	NA	Calibrated (-0.3 to 0 for Arg. and -0.39 to 0 for Q.)	-0.009 [-0.15; 0] (Arg.) -0.22 [-0.35; -0.14] (Q.)
С	Intercept of δ <sup>18</sup> O <sub>P</sub>	‰	Fixed	-10.0 (Arg.) -11.9 (Q.)

Table 2 Climate input data for all tested simulations

	Daily Tmin and Tmax	Daily P	Daily δ <sup>18</sup> O <sub>P</sub>	$CO_2$	
Configuration 1	Canadian database/ NOAA-CIRES dataset Linear regression				
Configuration 2	Canadian database / NOAA-CIRES dataset MUGCM data		GCM data	Loa	
Configuration 3	LMDZ-NCEP20 data				

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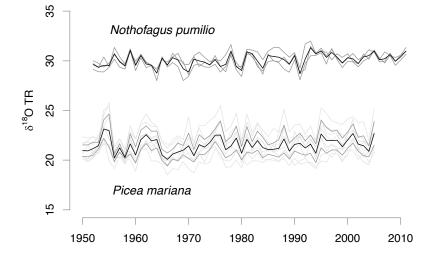
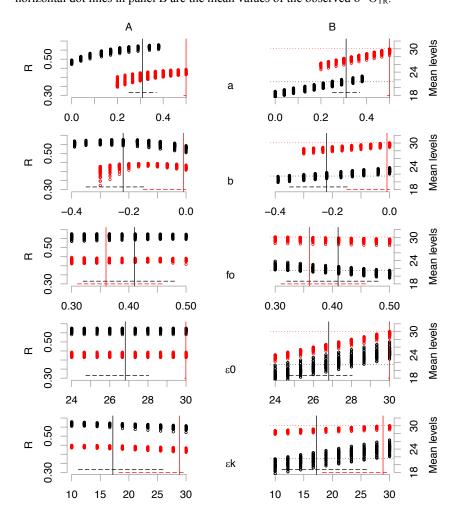


Figure 2 Dependence of the correlation coefficients between observed and simulated  $\delta^{18}O_{TR}$  series (panels A), and of the mean simulated  $\delta^{18}O_{TR}$  levels (‰) (panels B) as a function of the range of calibrated parameters a, b,  $f_o$ ,  $\epsilon_0$  and  $\epsilon_k$  for the 50 simulations performed. The tests sites from Quebec are in black and the Argentinean ones are in red. The vertical lines are the values of a plausible block of parameters retained in the MCMC optimization. The horizontal dashed lines are their respective 90% confidence interval calculated with 50 simulations (see Table 1). The horizontal dot lines in panel B are the mean values of the observed  $\delta^{18}O_{TR}$ .



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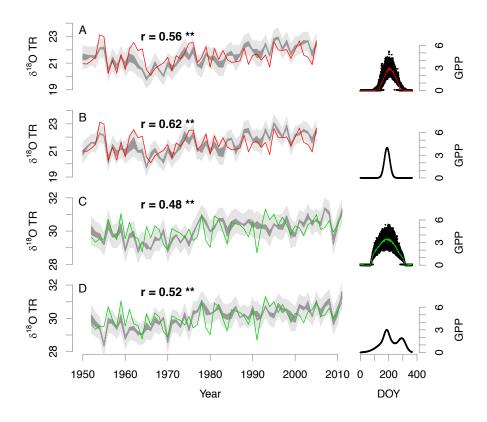
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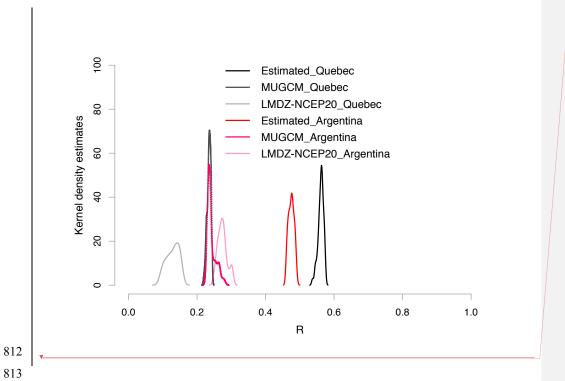
Figure 3 Comparison between observed (red or green) and simulated (grey)  $\delta^{18}O_{TR}$  chronologies in Quebec (A and B) and Argentina (C and D), respectively, using GPP (in gC.m<sup>-2</sup>.day<sup>-1</sup>) simulated by MAIDENiso for each day of the year (DOY) (A and C) or synthetized for maximizing correlations (B and D). The simulations are based on estimated  $\delta^{18}O_P$  series. The 50 different simulations inferred from the Markov Chain Monte Carlo (MCMC) chains are in dark grey. The  $\pm$  1 root mean square error (RMSE) range is represented in light grey. The mean correlation coefficients are significant at 99% level (\*\*).



**Figure 4** <u>Density distributions</u> of the coefficient of correlation (R) between observed and simulated  $\delta^{18}O_{TR}$  chronologies in Quebec and Argentina when the simulations are based on  $\delta^{18}O_P$  series estimated by the regression model or from the MUGCM and LMDZ-NCEP20 models.

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