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2 **Global-Scale Proxy System Modeling of Oxygen Isotopes in Lacustrine Carbonates:**  
3 **new insights from isotope-enabled-model proxy-data comparison**  
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14 **Abstract**

15 Proxy System Modelling (PSM) is now recognised as a crucial step in comparing climate model  
16 output with proxy records of past environmental change. PSMs filter the climate signal from the  
17 model, or from meteorological data, based on the physical, chemical and biological processes of  
18 the archive and proxy system under investigation. Here we use a PSM of lake carbonate  $\delta^{18}\text{O}$  to  
19 forward model pseudoproxy time-series for every terrestrial grid square in the SPEEDY-IER  
20 isotope enabled General Circulation Model (GCM), and compare the results with 31 records of lake  
21  $\delta^{18}\text{O}$  data from the Americas in the NOAA Paleoclimate Database. The model-data comparison  
22 shows general patterns of spatial variability in the lake  $\delta^{18}\text{O}$  data are replicated by the combination  
23 of SPEEDY-IER and the PSM, with differences largely explained by known biases in the models.  
24 The results suggest improved spatial resolution/coverage of climate models and proxy data,  
25 respectively, is required for improved data-model comparison, as are increased numbers of higher  
26 temporal resolution proxy time series (sub decadal or better) and longer GCM runs. We prove the  
27 concept of data-model comparison using isotope enabled GCMs and lake isotope PSMs and  
28 outline potential avenues for further work.  
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31 **Keywords**

32 Climate Variability; Lake Sedimentary Archives; Oxygen Isotopes; Proxy System Models; Isotope-  
33 Enabled GCMs

34

35 **Highlights**

- 36
- This paper presents the first global-scale forward modelling of lake carbonate  $\delta^{18}\text{O}$ .
  - 37 • The proxy system model accounts for lake water and isotope balance, and converts lake  
38 water isotope values to a predicted carbonate  $\delta^{18}\text{O}$  value.
  - 39 • Forward modelled lake carbonate  $\delta^{18}\text{O}$  is compared to a suite of available proxy data for  
40 the Americas, indicating moderate agreement between climate model and proxy data in  
41 terms of spatial trends.
  - 42 • Data-model comparison proves the concept and approach used, with differences largely  
43 explained by known model biases.
  - 44 • The new PSM provides avenues for future work comparing large proxy databases with  
45 isotope-enabled climate model simulations, as well as in paleoclimate data assimilation  
46 efforts.

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## 52 **1. Introduction**

53 Changes in water availability, driven in part by changing hydroclimate, have been shown to have  
54 impacts on societies past (e.g. Cullen et al., 2000) and present (e.g. Kelley et al., 2015), and will  
55 inevitably impact the future (IPCC, 2014). Understanding the spatial and temporal patterns of  
56 hydroclimatic change and their forcings is therefore of paramount importance for planning for  
57 potential future changes in water resources (IPCC, 2014). To this end, the last two thousand years,  
58 and last millennium in particular (PAGES Hydro2k Consortium, 2017), provide invaluable data for  
59 investigating hydroclimate variability at scales useful for human populations at frequencies difficult  
60 to establish using the instrumental record. The spatial and temporal resolution of both paleoclimate  
61 proxy records, e.g. annual PDSI reconstructions from tree rings (Cook et al., 2016), and climate  
62 models (e.g. Jungclaus et al., 2017) run using the same configurations as those for historic and  
63 future projections, through the last two millennia (PAGES Hydro2k Consortium, 2017) also allows  
64 for improved proxy-data climate-model comparison (data-model comparison hereafter). This  
65 comparison is important for quantitatively constraining future climate projections, by expanding the  
66 test bed for climate models beyond the instrumental period, but also for iteratively improving our  
67 proxy data interpretations and climate model skill.

68 One such proxy is the ratio of stable isotopes of oxygen, a useful tracer of the hydrological  
69 cycle that preserves in multiple geological archives, the analysis of which is now commonplace.  
70 The long term monitoring programme of the Global Network for Isotopes in Precipitation  
71 (IAEA/WMO, 2018) and its analysis (Dansgaard, 1964; Bowen and Wilkinson, 2002), and studies  
72 at finer spatial scales (e.g. Good et al., 2014; Tyler et al., 2016) allow isotopic patterns in  
73 precipitation to be recognised and understood in the present day, and the range of archives that  
74 preserve a function of these patterns in the past potentially allows a long and spatially broad record  
75 of changes in hydroclimate through time to be reconstructed.

76 Lakes can provide long and continuous terrestrial records of past oxygen isotope change  
77 (usually reported using the delta notation,  $\delta^{18}\text{O}$ ) and have a relatively good global coverage (e.g.  
78 Viau and Gajewski, 2001).  $\delta^{18}\text{O}$  can be measured from a range of hosts within the sediment  
79 archive including cellulose, diatoms, and a range of carbonate hosts such as ostracods,  
80 gastropods and sedimentary carbonate ( $\delta^{18}\text{O}_{\text{carb}}$ ). Cellulose is generally considered to be a direct

81 proxy of lake water isotope values ( $\delta^{18}\text{O}_i$ ; e.g. Wolfe et al., 2007) whereas  $\delta^{18}\text{O}_{\text{carb}}$  and  $\delta^{18}\text{O}_{\text{diatom}}$   
82 are functions of lake water temperature as well as  $\delta^{18}\text{O}_i$  (e.g. Dean et al., 2018). At a first order  
83 lakes can provide i) a direct measurement of  $\delta^{18}\text{O}_p$  or ii) the balance between precipitation amount  
84 and evaporation through time, depending on the hydrological setting of the lake (e.g. Leng and  
85 Marshall, 2004; Leng et al., 2006). However, there are multiple potential controls on  $\delta^{18}\text{O}_i$  (e.g.  
86 Jones et al., 2005) and the actual controls will be specific for any given lake at a particular time.  
87 Process studies monitoring the isotopic systematics of a given lake (e.g. Jones et al., 2016; Cui et  
88 al., 2018) can aid understanding and thereby interpretation of downcore isotope records from an  
89 individual site (e.g. Steinman et al., 2010). Furthermore, the use of isotope mass balance models  
90 (such as the one employed in this study) can lead to quantification of these interpretations.

91 Lake isotope mass balance models are an example of a Proxy System Model (PSM), a  
92 forward process-driven model of all or part of the climate-archive-proxy system (e.g. Evans et al.,  
93 2013). The PSM mathematically approximates biological, geochemical, and physical changes that  
94 the proxy system itself imparts on the measured proxy signal. PSMs for multiple proxy types have  
95 been published in recent years, particularly for high-resolution (e.g. tree ring width) and water-  
96 isotope based systems (ice cores, corals, tree cellulose and speleothems) (Tolwinski-Ward et al.,  
97 2011, Evans et al., 2013; Dee et al., 2015a). These models have demonstrated their usefulness  
98 and flexibility, facilitating studies which enhance interpretation of climate signals recorded by proxy  
99 data (e.g. Anchukaitis et al., 2006; Baker et al., 2012; Steinman et al., 2013), diagnosing the  
100 specific impacts of proxy system processes on the final measurement (Dee et al., 2015a),  
101 improving data-model comparison by placing models and paleoclimate observations in the same  
102 reference frame or in the same units (e.g. Thompson et al., 2011, Dee et al., 2017), providing a  
103 critical and more physically-based step in paleoclimate data assimilation (Steiger et al., 2014, Dee  
104 et al., 2016), and in tracking uncertainties inherent to different proxy types (Dee et al., 2015a).  
105 PSMs provide an improved and quantifiable understanding of how proxies filter the input climate  
106 signal and subsequently encode it in a paleoclimate measurement.

107 Building upon previous work, we present here a forward model of intermediate complexity  
108 for  $\delta^{18}\text{O}_i$  and  $\delta^{18}\text{O}_{\text{carb}}$ ; the model is applicable globally, and adaptable to individual sites if needed.  
109 The forward model program and example input are publicly available (<https://github.com/sylvia->

110 [dee/PRYSM](#)) and coded in R (R Core Team, 2016), an open-source and free computational  
111 platform. Given that lake isotope PSMs have been shown to do a good job of predicting monitored  
112 lake water isotope values for individual sites (e.g. Jones et al., 2016) this paper aims to investigate  
113 the effectiveness of more generic PSMs, and their potential in allowing lake  $\delta^{18}\text{O}$  records to be  
114 used as a data-model comparison tool. We first review previous work developing PSMs for  
115 isotopes in lacustrine archives (Section 2) and describe the model formulation and implementation  
116 for this study (Section 3). We demonstrate the efficiency and applications of this forward model,  
117 including data-model comparisons, using case studies of  $\delta^{18}\text{O}_{\text{carb}}$  in section 4. Section 5 concludes  
118 by reviewing the model's performance and discusses caveats and avenues for future work.

119

## 120 **2. Proxy System Modeling for Stable Water Isotopes in Lakes: a review**

121 Paleoclimatic proxies in lake sediments experience multivariate climatic controls (e.g. Jones et al.,  
122 2005) including, depending on proxy type, temperature, precipitation, evaporation, humidity, wind  
123 speed, and atmospheric circulation changes. The multivariate nature of the climatic forcings on  
124 lake sedimentary archives necessitates the use of PSMs which incorporate both the input climate  
125 and the processes that govern the proxy's recording of that climate signal. PSMs can explicitly  
126 connect climate variable inputs (modeled or observed) to the proxy measurement while accounting  
127 for the non-climatic influences on that measurement. In doing so, such transfer models help  
128 partition between the climate signal of interest and noise imparted by hydrological and/or  
129 geological processes. These PSMs, as forward models, can convert climate model simulations to  
130 pseudoproxy records (the mathematical proxy record produced by the PSM) and are now  
131 considered a fundamental step for robust data-model comparison (PAGES Hydro2k Consortium,  
132 2017).

133 Our PSM design follows previous work (Evans et al., 2013; Dee et al., 2015a) dividing the  
134 model into two different sub-components of the proxy system response to climate forcing, both of  
135 which serve a unique purpose: first, an *Environment Model* accounts for the impacts of the regional  
136 or local climatic impacts at the proxy measurement site; for lakes in particular, this includes the  
137 local hydrology of the lake system. Second, the *Sensor Model* describes the physical, geochemical  
138 and/or biological response of the proxy measured to environmental forcing.

139

140 *2.1 Environment Model: Hydrology & Lake Water Balance*

141 Isotope mass balance models have been used extensively to investigate lake hydrology (e.g.  
142 Dincer, 1968; Gat, 1995; Gibson et al., 2002) and quantitatively infer past climate change (Benson  
143 and Paillet, 2002; Jones et al., 2007; Steinman et al., 2010; Steinman et al., 2013). The models are  
144 based on variations of the following mass balance approach, where for a given, well-mixed, lake:

145

146 
$$dV/dt = P + Q_i - E - Q_o \tag{1}$$

147

148 where  $V$  is the lake volume,  $t$ , time,  $P$ , precipitation on lake surface per unit time,  $E$  is evaporation  
149 from lake surface per unit time and  $Q_o$  and  $Q_i$  are the sums of other outflows and inflows  
150 respectively, usually a combination of groundwater and surfacewater, measured in the same units  
151 as  $P$  and  $E$ .

152 The isotopic components of the lake must also similarly vary, for example in a lake where  
153 surface and groundwater inflows are meteoric water:

154

155 
$$\frac{d}{dt}(V\delta_i) = P\delta_P + Q_i\delta_P - E\delta_E - Q_o\delta_i \tag{2}$$

156

157 where  $\delta_P$ ,  $\delta_E$  and  $\delta_i$  are the isotope values of the precipitation, evaporation and lake waters  
158 respectively.

159  $\delta_E$  is difficult to measure and is therefore usually calculated (e.g. Steinman et al., 2010)  
160 using equations based on the evaporation model of Craig and Gordon (1965), for example:

161

162 
$$\delta_E = (\alpha^* \delta_i - h\delta_A - \epsilon)/(1 - h + (0.001\epsilon_k)) \tag{3}$$

163

164 where  $\alpha^*$  is the equilibrium isotopic fractionation factor dependent on the temperature at the  
165 evaporating surface e.g. as defined by Majoube (1971).  $h$  is the relative humidity normalised to the  
166 saturation vapour pressure at the temperature of the air water interface (e.g. Steinman et al., 2010)

167 and  $\epsilon_k$  is the kinetic fractionation factor e.g. as defined by Gonfiantini (1986).  $\delta_A$  is the isotopic  
168 value of the air vapour over the lake and  $\epsilon = \epsilon^* + \epsilon_k$  where  $\epsilon^* = 1000(1-\alpha^*)$ .

169  
170 *2.2 Sensor Model: Isotope Proxy Measurements from Lake Sediments*

171  $\delta^{18}\text{O}$  as a proxy can be measured from a range of hosts, so-called *sensors* within the PSM sub-  
172 model framework (Evans et al., 2013), within lake sediments (see introduction). Here we focus on  
173 lake carbonates.  $\delta^{18}\text{O}_{\text{carb}}$  is a function of  $\delta^{18}\text{O}_l$  and temperature, with the degree of temperature  
174 fractionation depending on the type of calcium carbonate precipitated in the lake waters. For  
175 calcite the fractionation between mineral and water ( $\alpha$ ) is expressed (Kim and O'Neil, 1997) as

176  
177 
$$1000 \ln \alpha_{(\text{calcite-water})} = 18.03(10^3T^{-1}) - 32.42 \quad (4)$$

178  
179 where T is temperature (K), whereas for aragonite (Kim et al., 2007)

180  
181 
$$1000 \ln \alpha_{(\text{aragonite-water})} = 17.88(10^3T^{-1}) - 31.14 \quad (5)$$

182  
183 Given seasonal variability in  $\delta^{18}\text{O}_l$  and temperature the timing of carbonate precipitation is  
184 therefore important. The timing of carbonate precipitation is a function of the concentration of  
185 bicarbonate and calcium ions in the lake waters, lake water temperature and pH (Kelts and Hsu,  
186 1978), which can be controlled by biological activity as well as physical changes in the lake system  
187 e.g. (Shapley et al., 2005). Isotopic measurements from biogenic carbonates can have additional  
188 species-specific vital effects, related to local  $\delta^{18}\text{O}_l$  values within lake sub-habitats, or additional  
189 fractionation effects during shell growth (e.g. van Hardenbroek et al., 2018).

190 For our work here we do not run modeled  $\delta^{18}\text{O}_{\text{carb}}$  through a model of sediment deposition  
191 that would take into account variability in the amount of carbonate precipitated in a given year, or  
192 sampling or chronological issues. PSM sub-models which account for chronological uncertainties  
193 and post-depositional effects such as bioturbation are forthcoming in companion and recently  
194 published work (e.g. Dee et al., in revision; Doman & Laepple, 2018).

195

196 **3. Methods**

197 Here, we present an adapted version of the forward model developed in Jones and Imbers (2010)  
198 and Jones et al. (2016) to model changes in  $\delta^{18}\text{O}_l$  and  $\delta^{18}\text{O}_{\text{carb}}$ , specifically from authigenic calcite.  
199 We drive a simplified version of this lake isotope forward model with output from the isotope-  
200 enabled atmospheric GCM, SPEEDY-IER (Dee et al., 2015b) using R. The R script used to  
201 generate the pseudoproxy data discussed here is given in the Supplementary Information and is  
202 available from <https://github.com/sylvia-dee/PRYSM>.

203 The analysis presented in this work requires a GCM simulation of sufficient length to  
204 assess decadal- to centennial-scale variability, sufficient resolution to provide sub-annual  
205 timesteps, as well as embedded water stable isotope physics. While other higher resolution  
206 isotope-enabled GCMs may offer a more advanced representation of atmospheric dynamics, most  
207 of these models are computationally expensive, and have not yet performed publicly available last-  
208 millennium simulations with water isotopes. SPEEDY-IER is an intermediate complexity  
209 atmospheric GCM (at resolution T31 or 3.75 x 3.75 degrees), and is a relatively efficient option for  
210 long paleoclimate integrations. Despite some simplifications to the model's physics, SPEEDY-IER  
211 simulates climatic and water isotope fields that are comparable with higher-order AGCMs at a  
212 much lower computational cost. For this study, SPEEDY-IER was forced with sea surface  
213 temperatures from the last millennium simulation (Landrum et al., 2013) of the CCSM4 coupled  
214 model (Gent et al., 2011), spanning 850-2005 AD; we extracted monthly data from model years  
215 1000-2005 AD for this study.

216 For the PSM's *Environment* sub-model, we assume a relatively straightforward lake  
217 hydrology, where the isotopic values of all water entering the lake (i.e. precipitation, groundwater  
218 and surface waters) is meteoric, and a minimum amount of inflow or outflow is required to maintain  
219 a lake in the basin given changes in evaporation and precipitation. Model lakes have a simple  
220 morphology such that lake area does not change with lake volume.

221 As a first-principles experiment, we forward model  $\delta^{18}\text{O}_l$  records at monthly time steps for a  
222 theoretical lake in every terrestrial grid cell in the climate model for the duration of the model run.  
223 We model a lake at each end of the hydrological gradient i.e. a fully open and fully closed lake,



224 thereby modelling the potential range of  $\delta^{18}\text{O}_{\text{carb}}$ , acknowledging that most lakes will lie somewhere  
225 between these two extremes.

226

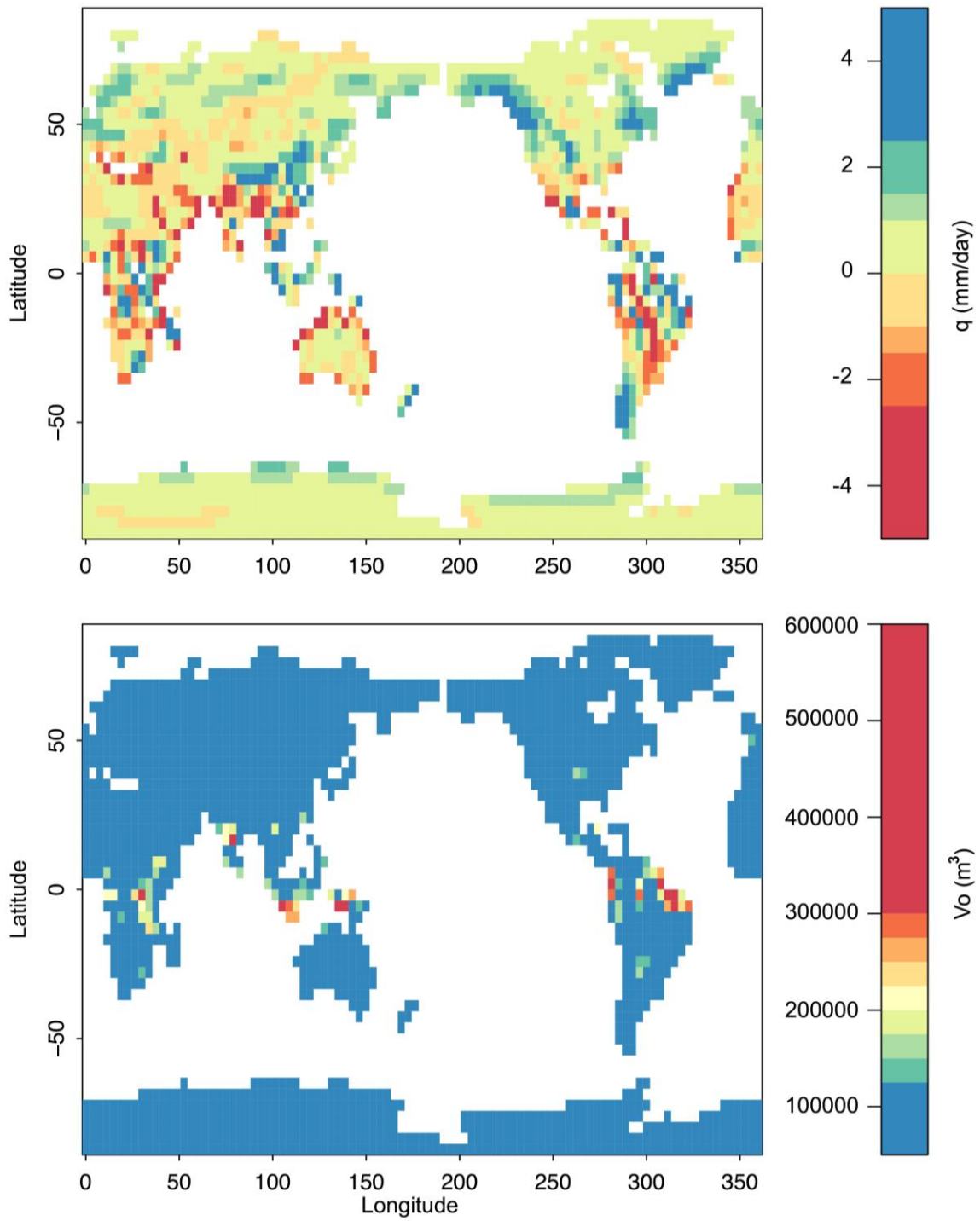
### 227 3.1 Forward Model Inputs: Hydrology

228 The hydrology, i.e. non isotopic components, of modelled lakes must also balance. For open lakes,  
229 with negligible evaporative control, we keep volumes constant for each monthly time step, with  
230 lake outflows equivalent to monthly inputs, taken here as twice the monthly precipitation value, to  
231 account for on lake and catchment inputs (see R code in Supplementary Information).

232 For closed lakes, in addition to the precipitation and evaporation components available  
233 directly from the climate model a ground-/surface-water component is also required. For a given  
234 lake, this component (Q) must be equal to P-E over the study period for the lakes to remain in near  
235 steady state (i.e. so the lake doesn't disappear or become unrealistically deep), such that for lakes  
236 in grid squares where  $P > E$ , Q will be positive and represent outflow, and where  $E > P$ , Q is negative  
237 and represents some inflow to the system. The value of P-E for a given grid square is therefore an  
238 important first-order control on the modeled lake hydrological balance. Here we calculate Q,  
239 indicating inflow vs. outflow, (see R code in the Supplementary Information) as a monthly constant  
240 based on the mean precipitation and evaporation values, from SPEEDY-IER, through the study  
241 period (Fig. 1a). Prior to use in the model any negative values of evaporation from SPEEDY-IER  
242 are replaced by values of 0.5 mm/day; values of 0 do not work for the forward model equations.

243 Lake volumes can then be calculated, from an initial starting point, for each monthly time  
244 step of the model. Initial lake volumes are based on a relatively small lake, with an area of 12,500  
245  $\text{m}^2$  and a depth of 8m. To ensure a lake continues to exist in each grid square throughout the study  
246 period, initial volumes ( $V_0$ ) for each grid square are recalculated if required after an initial run such  
247 that volumes for all grid squares are always above zero throughout the last millennium (Fig. 1b).

248 A useful byproduct of any lake isotope mass balance model, which requires a correct  
249 estimate of changing volume, is therefore a direct simulation of lake volume change through time,  
250 which can provide a useful metric for further data-model comparison for an individual lake system  
251 (e.g. Jones et al., 2016), or in the context of syntheses of lake level change (e.g. Street-Perrot et  
252 al., 1989, Hostetler & Bartlein, 1990).



254

255 **Figure 1** Mean annual values of  $q$  (p-e) and initial lake volumes ( $V_o$ ) for all terrestrial SPEEDY-IER  
 256 grid squares.

257

258 *3.2 Forward Model Inputs: Isotopes*

259 Initial values of  $\delta_i$  are based on the mean values of  $\delta_P$  from the full model time window. SPEEDY-  
260 IER's simulation of precipitation isotopes closer to the poles is limited by errors in the ability of the  
261 spectral dynamical core to advect very low humidity values; this leads to water isotope ratios in  
262 vapor and precipitation that are positively biased compared to observations. As a result, modelled  
263  $\delta^{18}\text{O}_P$  at the poles are too positive in SPEEDY-IER compared to GNIP data (Dee et al., 2015b),  
264 by up to 10-15‰ at the highest latitudes. We correct for this here by using the relationship between  
265 bias and temperature poleward of 30° described in Dee et al (2015b).

266 For the additional components needed for the closed lake systems,  $\delta_A$  is taken directly from  
267 SPEEDY-IER. It is recognised (e.g. Gibson et al., 2016; Lacey and Jones, this issue) that large  
268 lakes will impact their own hydrology, including changing values of  $\delta_A$  to include components of the  
269 evaporating lake waters. This is unlikely to impact the small basins modelled here, but would  
270 impact model-data comparison for larger lake sites if not accounted for. Lake inflow in months with  
271 no precipitation are given mean  $\delta_P$  values for that grid square.

272 Relative humidity and temperature values were extracted directly from SPEEDY-IER. Given  
273 known terrestrial temperature biases on the order of +1-3°K in SPEEDY-IER (Dee et al., 2015b)  
274 we use a temperature bias correction of -2°K for all grid squares. Lake temperatures also often  
275 differ from air temperatures above the lake (e.g. Sharma et al., 2008), and the difference between  
276 these temperatures is an important control on  $h$ . Based on 341 measurement of summer lake  
277 temperatures, measured by satellite or *in situ*, compared to air temperatures from the National  
278 Centres for Environmental Prediction (NCEP) and the Climatic Research Unit (CRU) in a global  
279 database (Sharma et al., 2015) lake temperatures are, on average, 1.5 degrees warmer than air  
280 temperatures (mean values of +1.4 for comparisons with NCEP data and +1.6 when compared to  
281 CRU). Although there is variability around this mean value, including lakes with cooler water  
282 temperatures than air temperatures, there are no clear spatial (latitude, longitude, altitude) or  
283 morphological (lake volume, surface area or maximum depth) controls on the difference between  
284 lake and air temperatures in the database such that we take the average of +1.5 degrees for all  
285 lakes modelled here. Values of  $h$  are then calculated following Steinman et al. (2010); see R code  
286 for details.

287 Values of the equilibrium ( $\alpha^*$ ) and kinetic ( $\epsilon_k$ ) fractionation factors are calculated from the  
288 corrected temperature and  $h$  values following the equations of Majoube (1971) and Gonfiantini  
289 (1986) respectively. With high relative humidity values the resulting values of  $\epsilon_k$  change sign,  
290 impacting calculations of  $\delta_E$ , such that  $h$  values were capped at 98%. Values of  $\delta_i$  for each time  
291 step for each grid square can then be calculated following the model equations from Jones et al.  
292 (2016); see R code in the Supplementary Information.

293

### 294 3.3 Sensor Model

295 Values for  $\delta^{18}\text{O}_{\text{carb}}$  were then calculated based on the calcite temperature fractionation equation  
296 (equation 4) of Kim and O'Neil (1997) using the rearrangement of this equation from Leng and  
297 Marshall (2004). Classical authigenic lake carbonates typically precipitate in summer months (e.g.  
298 Dean et al., 2015) following late spring algal blooms and/or ion concentration due to evaporation  
299 and here we calculate an annual value of  $\delta^{18}\text{O}_{\text{carb}}$  for the lake in each SPEEDY-IER grid square  
300 based on  $\delta_i$  and temperature values for January and June for southern and northern hemisphere  
301 lakes respectively.

302

## 303 4. Results and Discussion: Data-Model Comparison for Lake Carbonate Systems

304 Straightforward comparisons between climate model output and proxy observation is confounded  
305 by a number of uncertainties, outlined, for example, in Ault et al. (2013). First, the impacts of the  
306 proxy system itself on the measured signal, potentially unrelated to climate, must be accounted for.  
307 We address this directly with the construction of the lake carbonate PSM presented in this work,  
308 but acknowledge the relatively low level of complexity in the PSM used. The PSMs used here  
309 restrict the hydrological complexity of the model lakes; the degree of hydrological closure of a given  
310 lake can impact its isotopic sensitivity to climate change for example (Jones and Imbers, 2010). In  
311 general, however, these potential PSM biases are site specific, and are therefore not possible to  
312 generalise for a model applied at the global scale. We would take a different approach, using a  
313 more complex PSM if the aim of our study was to compare an individual site, or a small group of  
314 sites, to climate model output, rather than the global-scale view employed here.

315 Second, climate models contain biases, and simulate internal variability which is inherently  
316 different from that recorded by paleoclimate data (e.g. Dee et al., 2017). We have discussed  
317 known biases in SPEEDY-IER, and how these have been accounted for in this study in the  
318 previous section, and discuss variability later in the paper. In addition, as with other GCMs,  
319 SPEEDY-IER's grid cells of 3.75 degrees, equating to approximately 176,400 square kilometers,  
320 dwarf the often-microclimate scale of the lakes. Due to these limitations, of both PSMs and GCMs,  
321 we therefore do not expect that point-based comparisons can necessarily yield meaningful  
322 information about model-data agreement nor fully inform model-data discrepancies, however  
323 global scale trends should still be evident.

324 We have circumvented these challenges where possible by translating the climate model  
325 output to proxy units using the PSM, and comparing time-scale dependent variances and broad  
326 spatial trends in both the model and data, rather than looking for direct site-grid square  
327 comparisons. The data used are extracted from the NOAA Paleoclimate Database  
328 (<https://www.ncdc.noaa.gov/data-access/paleoclimatology-data>). We extracted relevant data by  
329 searching with the query *Paleolimnology > oxygen isotopes* between the years 1000 to -50 cal  
330 years BP. This resulted in 53 available data sets. 41 of these are from the Americas, with only 3  
331 from Europe and Africa, so we focus here on the Americas for data model comparisons to  
332 maximize our ability to use as large a range of data sites as possible, whilst having some  
333 constraint on space given global isotopic and climatic gradients. Of these 41 datasets, we removed  
334 records from non-carbonate hosts, such as diatoms, resulting in a final dataset of 31 lake sites with  
335  $\delta^{18}\text{O}_{\text{carb}}$  data records to compare with the pseudoproxy data sets (Table 1).

336

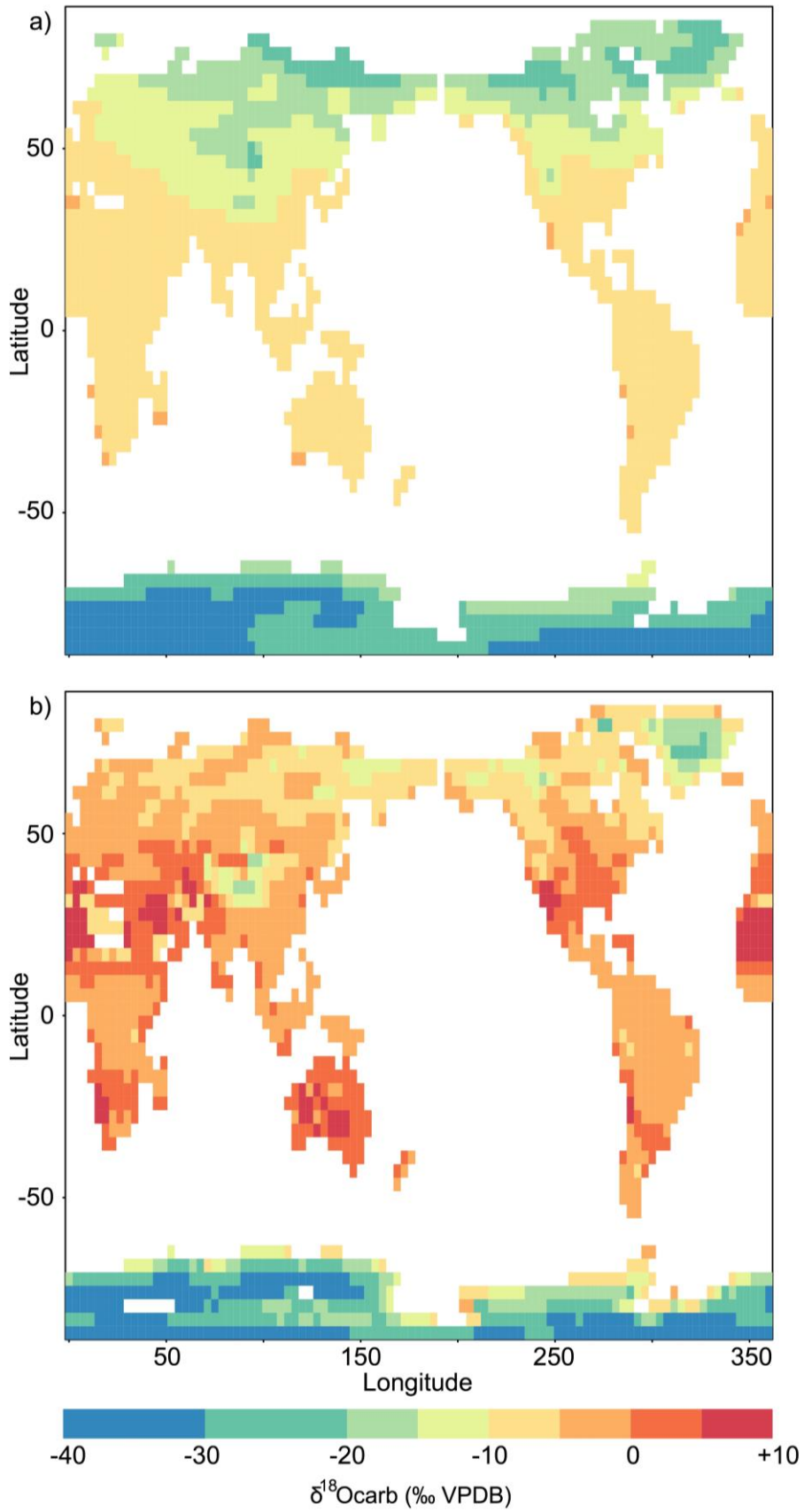
#### 337 *4.1 Spatial variability*

338 Figure 2 shows the mean annual  $\delta^{18}\text{O}_{\text{carb}}$  simulated by the open and closed lake PSMs in each  
339 terrestrial GCM grid cell. In agreement with theory, the forward-modeled lakes indicate more  
340 evaporative enrichment of  $\delta^{18}\text{O}_{\text{carb}}$  in the subtropics (e.g. Australia, the Southwestern U.S.) and  
341 more depleted  $\delta^{18}\text{O}_{\text{carb}}$  values in the tropics (e.g. Amazon & Congo basins) and toward the poles.  
342 The open lake PSM results which reflect the weighted average of  $\delta_{\text{p}}$ , show the general trend  
343 towards more negative isotopic values of precipitation at the poles and more continental areas

344 (Bowen and Wilkinson, 2002). The greater divergence between open and closed lakes at mid  
345 latitudes (c. 30° N and S) would be expected given evaporation is more often a control of lake  
346 isotope records, resulting in more positive values of  $\delta_l$  and  $\delta^{18}\text{O}_{\text{carb}}$ , at these latitudes (e.g. Roberts  
347 et al., 2008).

348 To evaluate and compare spatial variability in the model and the data directly, Figure 3  
349 compares lake isotope data from the Americas with the latitudinal patterns evident in the forward  
350 model results. If the SPEEDY-IER model variable output and the PSM's subsequent simulation of  
351  $\delta^{18}\text{O}_{\text{carb}}$  agree with observations, most lake carbonate data through the last millennium should fall  
352 between the blue and green lines in Fig. 3, representing open and closed lakes. This comparison  
353 shows that the general spatial trends of lake  $\delta^{18}\text{O}_{\text{carb}}$  data, particularly the latitudinal gradient, are  
354 well simulated by the PSM and SPEEDY-IER.

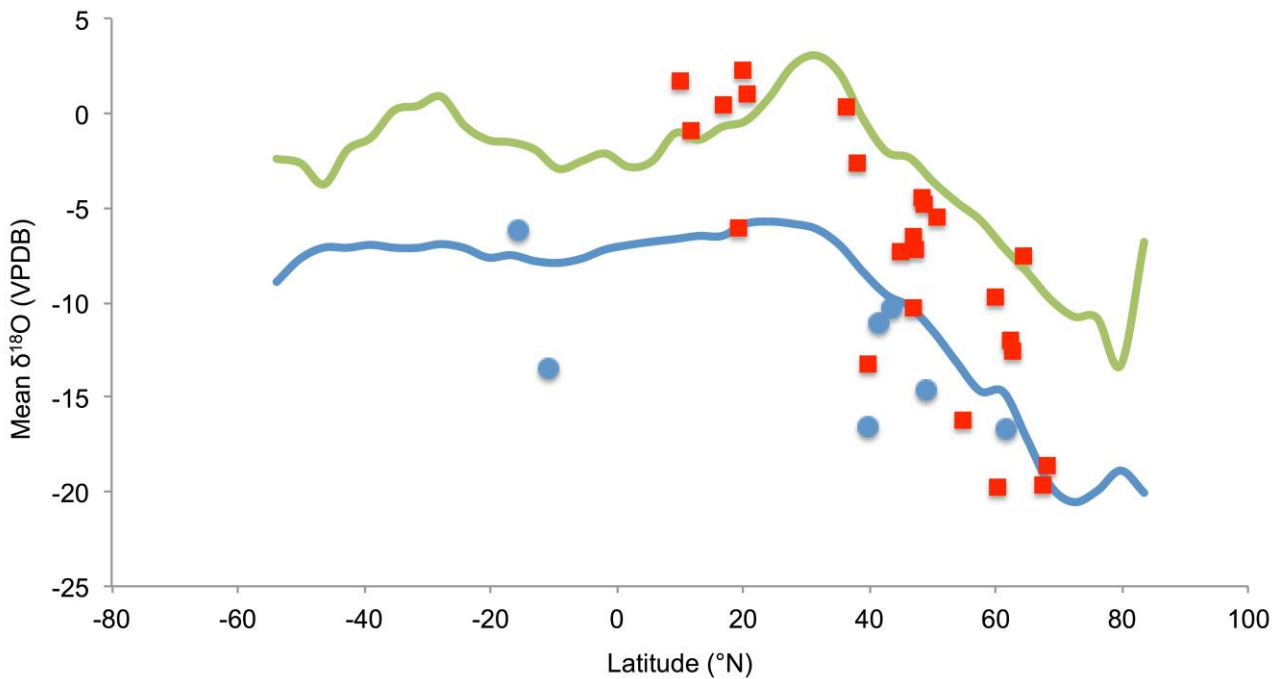
355 To look at the data-model differences in more detail we compared proxy data and  
356 pseudoproxy time-series from the 12 sites amongst our 31-site data list that have temporal  
357 resolution approaching that of SPEEDY-IER i.e. more than one data point per 10 years (Fig. 4).  
358 For the open lakes Lime Lake data shows similar values to the open lake PSM, as does Martin  
359 Lake for some parts of the record (Fig. 4). The large range of  $\delta^{18}\text{O}_{\text{carb}}$  values from the Martin Lake  
360 core are driven by changes in the dominant rainfall source area through the record (Bird et al.,  
361 2017). The PSM-data comparison suggest here that SPEEDY-IER does a good job of  
362 reconstructing  $\delta^{18}\text{O}_p$  values similar to present day, but does not reconstruct the dramatic changes  
363 in rainfall source area related to the Pacific North American pattern recorded by the Martin Lake  
364 sediments. Data-PSM comparison of Steel Lake also suggests a good match, with the  $\delta^{18}\text{O}_{\text{carb}}$   
365 values closely matching the open lake PSM pseudoproxy values (Fig. 4). However, Tian et al.  
366 (2006) interpret the core data from Steel Lake as being influenced by evaporation, due to some  
367 isotopic measurements of modern lake waters and calibration of recent sediment  $\delta^{18}\text{O}_{\text{carb}}$  with P-  
368 AET measurements. The lake is described as having a small stream running through it and having  
369 some groundwater influence, such that evaporation may be less influential than described,  
370 however it also possible that the  $\delta^{18}\text{O}_p$  bias correction applied here to SPEEDY-IER at higher  
371 latitudes is not sufficient at Steel Lake (46°58'N), such that the pseudoproxy data for both open  
372 and closed lakes are too positive.



374

375 **Figure 2** Mean annual carbonate values simulated from a) open and b) closed lake forward

376 models in each SPEEDY-IER grid square for the last millennium.



378

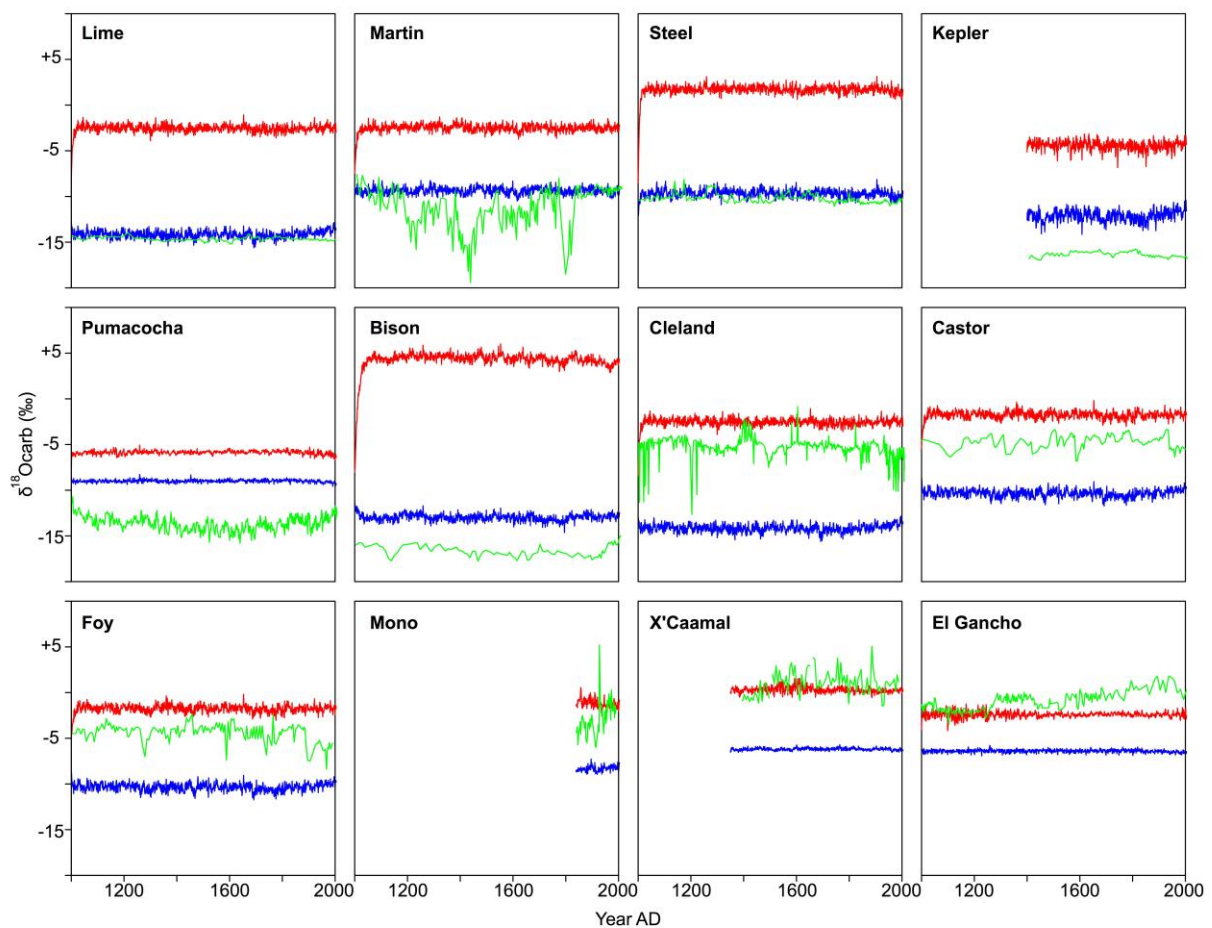
379 **Figure 3** Comparison of latitudinal patterns in  $\delta^{18}\text{O}_{\text{carb}}$  in the Americas from forward modelled open  
 380 (blue) and closed (green) lakes compared to data from the NOAA Paleoclimate Database (Table 1)  
 381 from both open (blue circles) and closed (red squares) lakes.

382

383 Three other open lake sites do have  $\delta^{18}\text{O}_{\text{carb}}$  data more negative than the open lake PSM  
 384 pseudoproxy data. Pumacocha and Bison Lake are extremely high elevation sites compared to the  
 385 others shown in Figure 4 (4300 and 3255 m.a.s.l. respectively). Topography in SPEEDY is not well  
 386 resolved so there are known biases in capturing the full amount effect (Dee et al., 2015b) that  
 387 could not be systematically corrected for here. Kepler Lake is the highest latitude site (61.6°N) of  
 388 the twelve shown in Fig. 4. It is possible that the negative data offset compared to the open lake  
 389 PSM here is therefore due to an underestimation of the latitudinal bias correction used, as  
 390 suggested for Steel Lake. There are also potential hydrological reasons that could cause this  
 391 offset, with high latitude and high altitude sites potentially more impacted isotopically by snow melt,  
 392 which would likely lead to a negative isotope bias compared to a direct precipitation input to the  
 393 lake (e.g. Beria et al., 2018).



394 Cleland, Castor, Foy and Mono Lakes sit, as would be expected, within the theoretical end  
 395 member PSM lakes for their locations. The two remaining sites Aguada X'caamal and El Gancho  
 396 have data that are more positive than the closed lake pseudoproxy records (Fig. 4). This suggests  
 397 that inputs to the system are isotopically too negative in the PSM. SPEEDY-IER tends to have a  
 398 positive bias in  $\delta^{18}\text{O}_p$ , although more so at high latitudes, and there is relatively little GNIP data  
 399 through Latin America with which to compare models or data to. Another possibility is that water at  
 400 these sites is evaporated before entering the groundwater, e.g. in the soil, causing evaporative  
 401 enrichment that is not adequately represented in the PSM framework.



402  
 403 **Figure 4** Comparison of pseudoproxy time series from open (blue) and closed (red) lake PSMs  
 404 from the equivalent SPEEDY-IER grid squares of the 12 high resolution lake  $\delta^{18}\text{O}_{\text{carb}}$  data sets  
 405 (Table 1).

406  
 407 In summary, looking at the variance of lake isotope records in *space*, this work confirms  
 408 that first order lake PSMs coupled to an intermediate-complexity climate model can resolve

409 observed continental patterns in  $\delta^{18}\text{O}_{\text{carb}}$  data, whilst further informing our interpretation of some of  
410 these records, and helping to diagnose the impacts of biases in the climate model and PSM.

411

#### 412 *4.2 Temporal patterns and variability*

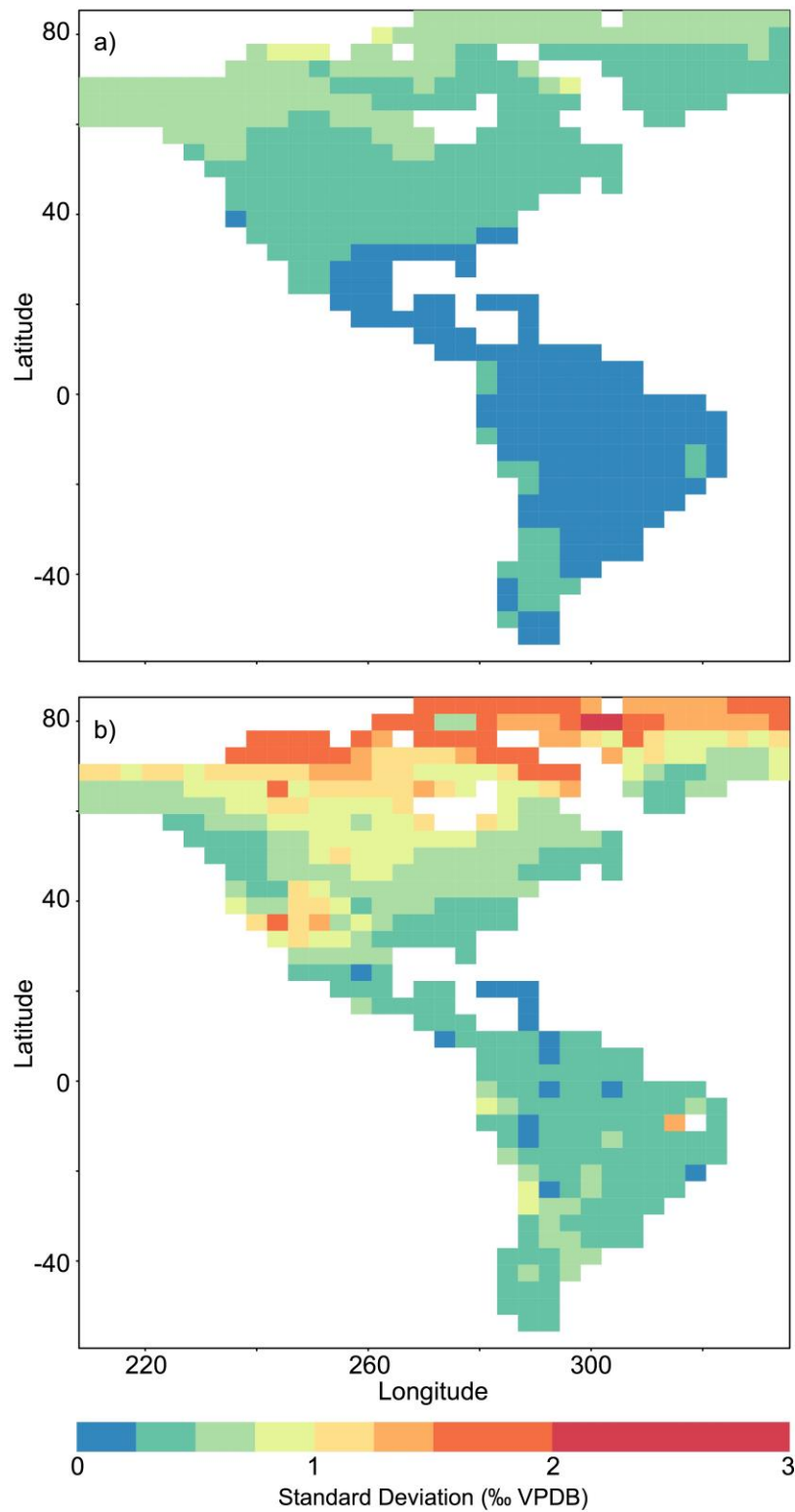
413 Recent work has highlighted the fact that even with the additional information provided by a proxy  
414 system model, observations from paleoclimate archives show larger temporal variability at decadal  
415 to centennial timescales than GCMs, and PSMs driven with their output, currently simulate  
416 (Laepfle & Huybers, 2014, Dee et al., 2017). This is evident in the records shown in Figure 4  
417 where the  $\delta^{18}\text{O}_{\text{carb}}$  data, even at lower resolution than the pseudoproxy records, tend to show  
418 greater variability, with the exception of some of the open lake records such as Kepler and Lime.

419 Greater variability in closed lakes, compared to open systems, is what would be expected  
420 from lake isotope theory (e.g. Leng and Marshall, 2004; Roberts et al., 2008) and previous  
421 modelling studies (Jones and Imbers, 2010). This is also evident in the PSM output here e.g.  
422 when comparing variability in open and closed lake  $\delta^{18}\text{O}_{\text{carb}}$  pseudoproxy records across the  
423 Americas (Fig. 5).

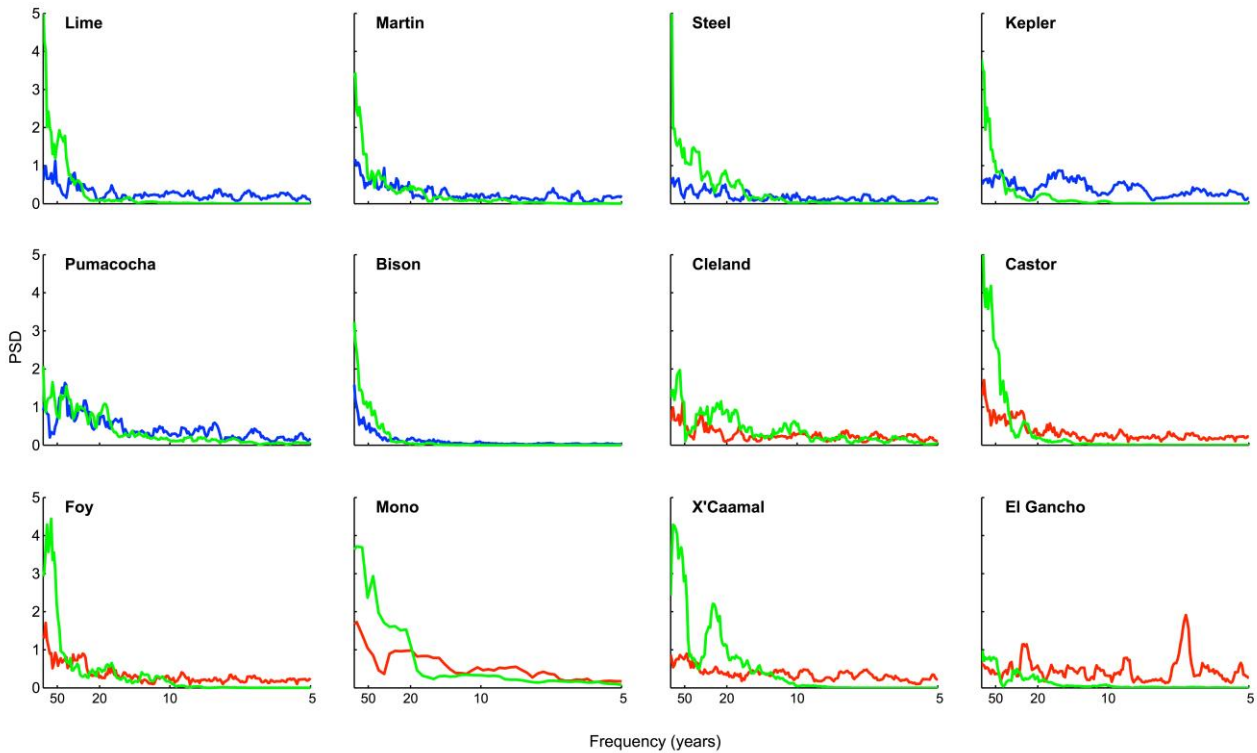
424 Comparing the power spectral densities (PSDs) between proxy and pseudoproxy data  
425 provides a way of comparing the dominant modes of variability in both time-series. We compare  
426 the 12 highly resolved data records and their pseudoproxy equivalent time-series in this way  
427 (Figure 6) using the open or closed PSM output where appropriate. Using this approach Dee et al.  
428 (2017) found that PSMs of a number of proxies, including speleothem and coral carbonates  $\delta^{18}\text{O}$ ,  
429 whilst helping to resolve model-data differences at interannual to decadal timescales, could not  
430 account for a mismatch in variance at multi-decadal to centennial timescales. Our results here tell  
431 a similar story.

432 In nearly all cases the proxy data show more power at lower frequencies compared to the  
433 pseudoproxy time series, with the pseudoproxy time series having more power at higher, sub-  
434 decadal, frequencies (Fig. 6). Exceptions to this are for Pumacocha, where the PSD curves are  
435 very similar for both data and pseudoproxy time series, and to some degree for Bison Lake. It is  
436 interesting to note that these two open sites, at high elevation, which have data more negative data

437 than the equivalent PSMs both show the closest match in term of temporal variability between the  
438 data and PSM output.  
439



440  
441 **Figure 5** Standard deviation of pseudoproxy  $\delta^{18}\text{O}_{\text{carb}}$  time series from a) open and b) closed lakes  
442 in each grid square in the Americas through the last millennium.



444

445 **Figure 6** Comparison of the power spectra from data and pseudoproxy time-series from open  
 446 (blue) and closed (red) lake PSMs. We estimate power spectra of the PSM pseudoproxy data and  
 447 the proxy data, interpolated to annual resolution, using Thomson's multi-taper method (Thomson,  
 448 1982).

449

450 Given their length and continuity lake records provide a potentially important check on  
 451 lower frequency climate modes simulated by GCMs. The comparisons here suggests that  
 452 resolving lower frequency variability observed in proxy data, with the exception here of some  
 453 higher elevation locations, remains a challenge for GCMs, even when filtered by a PSM. Further  
 454 work on PSM complexity may also help further understand this issue.

455

## 456 5. Summary

457 The work presented here further develops our understanding of forward modeling paleoclimate  
 458 archives; moving towards best practices in data-model comparison by creating physically-based  
 459 transfer functions to translate between the variables of climate model output and the multivariate

460 (and sometimes nonlinear) signals encoded in paleoclimate data (Evans et al., 2013, Dee et al,  
461 2015a).

462         Recent efforts to compile large, standardized databases of paleoclimate data spanning the  
463 last 2 millennia, beyond those employed in this work, and including, but not limited to Pages2k  
464 (PAGES 2k Consortium, 2017) and Iso2k (Konecky et al., 2017) are providing an invaluable new  
465 platform for the investigation of temporal, and spatial trends characterizing Earth's climate through  
466 the last two millennia. Alongside paleoclimate model intercomparison projects, such as PMIP3  
467 (Brannocot et al., 2011, 2012) and the forthcoming PMIP4 (Kageyama et al., 2016), they provide  
468 opportunities for large-scale data-model comparison to constrain hydroclimate variability in space  
469 and time. These comparisons will require PSMs for multiple proxy types and the approach  
470 introduced in this paper will help facilitate this further.

471         The approach in this paper may also facilitate broader use of lake data in paleoclimate data  
472 assimilation and paleoclimate reanalysis products (e.g. Steiger et al., 2014, Hakim et al., 2016,  
473 Dee et al., 2016). To date, these studies have only employed annually-resolved proxy data,  
474 however the framework for assimilating data unevenly spaced in time is operational (Malevitch et  
475 al., 2017). Thus, work such as that presented here provides a new link for the assimilation of lake  
476 sedimentary records in paleoclimate reanalyses.

477         We were limited here to just one isotope-enabled model simulation. SPEEDY-IER is an  
478 intermediate-complexity AGCM, and thus houses temperature and precipitation bias which  
479 influence the PSM's pseudoproxy output. Indeed, a PSM's output is inherently limited by the  
480 climate model or observational data used to drive the model. However, future work will examine  
481 whether higher-order isotope-enabled GCMs might improve comparisons with observations.  
482 Additional millennial-scale simulations which include water isotopes are becoming increasingly  
483 available, and we will repeat these experiments with higher-order GCM simulations and more  
484 complex lake PSMs to check the impacts of intermediate-complexity biases explicitly in future  
485 work. As more proxy data become available this will further increase the usefulness of such data-  
486 model comparisons, and work such as that presented here presents challenges to both data and  
487 model communities to improve the products available for data-model comparison, for example

488 GCMs that better simulate higher latitude  $\delta^{18}\text{O}_p$  or improving the spatial spread of proxy data  
489 available for comparison.

490 Lake sedimentary archives constitute one of the richest data sources for hydroclimatic  
491 reconstructions given their broad global coverage and temporal lengthscales. Characterizing  
492 climate variability on multi-decadal to centennial timescales from these archives is crucial for  
493 validating the 'slow-physics,' or low-frequency variability component in climate models, outside the  
494 relatively brief purview of 20th century observations. To this end, we hope that this work provides a  
495 step forward for extracting the most meaningful signals from lacustrine carbonates, with full  
496 appreciation for stable water isotope physics operating in the atmosphere, as well as lake  
497 hydrology. Data-model comparison techniques which account for confounding proxy system  
498 impacts will only strengthen our interpretations of these data, enhancing our understanding of  
499 processes occurring on the landscape and informing our interpretations of atmospheric variability  
500 as captured by the proxy data. Taken together, this information provides more robust constraints  
501 for climate model simulations of long-term variability, essential for useful future climate projections.

502

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510

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**Table 1** Lake carbonate records from the last millennium in the NOAA paleoclimate database used in this study. \*High resolution sites (see text for discussion).

Site Name	Latitude	Longitude	Mean $\delta^{18}\text{O}_{\text{carb}}$ (‰)	$\sigma$ $\delta^{18}\text{O}_{\text{carb}}$ (‰)	Lake Hydrology (Open/Closed)	Reference
<i>Keche</i>	68.02	-146.92	-18.57	0.71	Closed	Chipman et al., 2012
<i>Takahula</i>	67.35	-153.66	-19.70	1.73	Closed	Clegg and Hu, 2010
<i>Quartz</i>	64.20	-149.82	-7.50	0.91	Closed	Wooller et al., 2012
<i>Farewell</i>	62.55	-153.63	-12.55	0.13	Closed	Hu et al., 2001
<i>Seven Mile</i>	62.17	136.38	-11.99	0.59	Closed	Anderson et al., 2011
<i>Kepler*</i>	61.55	-149.20	-16.70	0.29	Open	Gonyo et al., 2012
<i>Jellybean</i>	60.35	-134.80	-19.76	0.33	Closed	Anderson et al., 2005
<i>Marcella</i>	60.07	-133.80	-9.71	1.02	Closed	Anderson et al., 2007
<i>Paradise</i>	54.69	-122.62	-16.26	0.40	Closed	Steinman et al., 2016
<i>Cleland*</i>	50.83	-116.39	-5.44	1.19	Closed	Steinman et al., 2016
<i>Lime*</i>	48.87	-117.34	-14.63	0.20	Open	Steinman et al., 2012
<i>Castor*</i>	48.54	-119.56	-4.80	0.71	Closed	Steinman et al., 2012
<i>Foy*</i>	48.17	-114.35	-4.49	1.02	Closed	Stevens et al., 2006
<i>Elk</i>	47.20	-95.25	-7.21	0.42	Closed	Anderson et al., 1993
<i>Jones</i>	47.05	-113.14	-6.49	0.71	Closed	Shapley et al., 2009
<i>Steel*</i>	46.97	-94.68	-10.29	0.47	Closed	Tian et al., 2006
<i>Crevice</i>	45.00	-110.58	-7.30	0.95	Closed	Whitlock et al., 2012
<i>Crawford</i>	43.47	-79.95	-10.30	0.88	Open	Yu and Eicher, 1998
<i>Martin*</i>	41.56	-85.38	-11.10	2.23	Open	Bird et al., 2017
<i>Bison*</i>	39.75	-107.33	-16.60	0.59	Open	Anderson, 2011
<i>Yellow</i>	39.65	-107.35	-13.28	0.44	Closed	Anderson, 2012
<i>Mono*</i>	38.00	-119.00	-2.64	1.57	Closed	Li et al., 1997
<i>Abbott</i>	36.23	-121.48	0.32	1.61	Closed	Hiner et al., 2016
<i>X'caamal*</i>	20.60	-88.28	1.06	1.28	Closed	Hodell et al., 2005
<i>Chichancanab</i>	19.88	-88.77	2.28	0.63	Closed	Hodell et al., 2001
<i>Aljojuca</i>	19.09	-97.53	-6.02	2.67	Closed	Bhattacharya et al., 2015
<i>Peten Itza</i>	16.92	-89.83	0.51	0.24	Closed	Curtis et al., 1998
<i>El Gancho*</i>	11.90	-85.92	-0.93	0.94	Closed	Stansell et al., 2013
<i>Valencia</i>	10.17	-67.75	1.75	0.54	Closed	Curtis et al., 1999
<i>Pumacocha*</i>	-10.70	-76.06	-13.44	0.68	Open	Bird et al., 2011
<i>Umayo</i>	-15.44	-70.10	-6.12	0.98	Open	Ekdahl et al., 2008