

1 **Quantifying closed-basin lake temperature and hydrology by**
2 **inversion of oxygen isotope and trace element paleoclimate records**

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11 **ABSTRACT. Lake systems are important paleoclimate archives that preserve ecosystem**
12 **and hydrologic responses to critical periods in Earth history, such as carbon cycle**
13 **perturbations and glacial-interglacial cycles. Geochemical measurements of biogenic**
14 **carbonate (for example, $\delta^{18}\text{O}$, $\delta^{13}\text{C}$, $^{87}\text{Sr}/^{86}\text{Sr}$, [Li], [U], [Sr], and [Mg]) are indicators of**
15 **hydrologic variability in lake systems throughout the geologic record. In this study, we**
16 **present a new closed-basin lake modeling approach, HyBIM (the Hydrologic Balance**
17 **Inverse Model), that employs a system of total differential equations and uses the measured**
18 **$\delta^{18}\text{O}$, Sr/Ca, and Mg/Ca of biogenic carbonate to determine changes in temperature, runoff,**
19 **and lake evaporation. Using equally-spaced time steps, these equations are simultaneously**
20 **solved to constrain the hydrologic parameters of the lake as recorded in biogenic carbonate.**
21 **We use a Monte Carlo approach to account for uncertainty in the input parameters, such**
22 **as $\delta^{18}\text{O}$ temperature relationships, partition coefficient uncertainty, and watershed solute**
23 **chemistry.**

24 **For illustrative purposes, we apply the model to two ostracod valve datasets**
25 **covering different timescales: (1) the Cretaceous Songliao Basin, northeast China, and (2)**
26 **Holocene Lake Miragoane, Haiti. Modern water measurements of water isotopes and**
27 **cation concentrations from each location are required as model inputs. We compare our**
28 **modeling results with author interpretations and geologic observations. The modeling**
29 **approach presented in this study can be applied to other closed-basin lake records, can be**
30 **modified for other calcifying species (for example, gastropods or mollusks) or with**
31 **calibration to inorganic lacustrine carbonate. In addition, this approach holds promise for**
32 **extension with additional proxy measurements (that is, δD , U/Ca or Li/Ca) and changing**
33 **source area on tectonic timescales using proxies that reflect changing source lithology (that**

57 investigated (for example, Nilsson, 1931; Eugster and Kelts, 1983; Kelts, 1988; Talbot, 1990;
58 Carroll and Bohacs, 1999). Within the Carroll and Bohacs (1999) framework, closed-basin lakes
59 are of two types: balanced-fill and underfilled. Underfilled lake systems are identified by
60 evaporative facies (Jones and others, 1977; Eugster and Jones, 1979; Horita, 1990) and are
61 typical of many Quaternary playa-lake systems found in semi-arid regions of the mid-latitudes,
62 such as the western United States (Mifflin and Wheat, 1979; Reheis and others, 2014). In
63 contrast, balanced-filled lake systems are typical of freshwater to saline conditions with mixed
64 carbonate and siliciclastic sediments (for example, Carrol, 1998; Kempf and others, 2009;
65 Doebbert and others, 2014).

66 For closed-basin Quaternary lake systems, in which tectonic rearrangement is negligible,
67 climatic conditions have been quantified using measures of lake surface area and tributary size
68 (Snyder and Langbein, 1962; Mifflin and Wheat, 1979; Bowler, 1981; Benson and Paillet, 1989;
69 Bengtsson and Malm, 1997; Reheis, 1999; Sack, 2009; Broecker, 2010; Munroe and Laabs,
70 2013; Hudson and Quade, 2013; Ibarra and others, 2014; Huth and others, 2015; Hudson and
71 others, 2015). Additionally, recent work modeling stable isotopes in closed-basin balance-filled
72 lakes takes advantage of longer (relative to overfilled/open lakes) residence times to infer
73 climatic conditions by relating the $\delta^{18}\text{O}$ or δD to the hydrologic balance (Horita, 1990; Hostetler
74 and Benson, 1994; Benson and White, 1994; Gibson and others, 2002; Gibson and Edwards,
75 2002; Benson and Paillet, 2002; Jones and others, 2007; Russell and Johnson, 2006; Jones and
76 Imbers, 2010; Doebbert and others, 2010; Steinman and others, 2010a,b; 2012; 2013; Steinman
77 and Abbott, 2013; Jasechko and others, 2013; Stansell and others, 2013; Ibarra and others, 2014;
78 Jasechko and others, 2014; Gibson and others, 2015). Fundamental to applying an isotopic
79 modeling approach are assumptions concerning the watershed precipitation-runoff relationships

80 (Jones and others, 2007; Ibarra and others, 2014), mixing or stratification of the lake (Imberger
81 and Ivey, 1991), basin-scale and regional vapor recycling (Gat and Matsui, 1991; Gat and others,
82 1994; Burnett and others, 2003; Winnick and others, 2014), and groundwater influences
83 (Krabbenhoft and others, 1990a,b; Shapley and others, 2005; Guay and others, 2006; Steinman
84 and others, 2013). While these models offer powerful methods to reconstruct the hydrology of
85 lake systems they are limited by the numerous input parameters required that are difficult to
86 constrain in ancient lake systems. Another approach, outlined here, is to use additional
87 measurements, such as trace elements, that can be meaningfully related to climatic conditions
88 and will reduce the assumptions necessary for accurate, quantitative climatic reconstructions.
89 Using trace element and oxygen isotope measurements it is then possible to tightly constrain the
90 system using far fewer input parameters.

91 In this paper, we develop a new modeling framework exploiting variations in $\delta^{18}\text{O}$ and
92 trace elements (Mg and Sr) measured in lacustrine carbonates and utilizing a series of total
93 differential equations. We apply this model to previously published ostracod paleoclimate
94 records for closed basins. Lacustrine ostracod records are used here for illustrative purposes
95 because of their broad paleoclimate applications in historical (for example, Engstrom and Nelson,
96 1991; Holmes and others, 2007a; Zhang and others, 2009), Quaternary (for example, Edney and
97 others, 1990; Hodell and others, 1991; Curtis and Hodell, 1993; Lamb and others, 1999; Cohen
98 and others, 2000; Holmes and others, 2007b; Gouramanis and others, 2010), and deep-time (for
99 example, Forester, 1991; Chamberlain and others, 2013) settings. Extensive work has also been
100 carried out on the ecology, taphonomy, and taxonomy of ostracod species (for example, Horne
101 and others, 2002; Frogley and others, 2002; Bennett and others, 2011; Blome and others, 2014),
102 and modern ostracod datasets have been extensively studied and provide the necessary empirical

103 calibrations of trace element distribution coefficients and vital effects (for example, Engstrom
104 and Nelson, 1991; Xia and others, 1997a,b; Wansard and others, 1998; De Deckker and others,
105 1999; Dettman and others, 2002; Holmes and Chivas, 2002; Dwyer and others, 2002; Ito and
106 Forester, 2009; Gouramanis and De Deckker, 2010; Marco-Barba and others, 2012; Börner and
107 others, 2013) necessary to constrain our model. The modeling framework presented in this paper
108 applies, given the existence of relevant and accurate calibrations, to any biogenic carbonate
109 records from a closed-basin lake setting.

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111 MODEL DEVELOPMENT

112 We present the Hydrologic Balance Inversion Model (HyBIM), an inverse model using a
113 system of total differential equations that are inverted to solve for the extensive variables in lake
114 chemistry. The structure of the model is similar to models that quantify changes in the global
115 carbon cycle and/or other biogeochemical cycles as recorded in marine sediments (for example,
116 Godd ris and Fran ois, 1996; Derry and France-Lanord, 1996; Fran ois and Godd ris, 1998; Li
117 and others, 2009; Li and Elderfield, 2013). We solve for the relative changes in temperature and
118 lake volume, and thus rely only on the first derivative of the input dataset and not the absolute
119 value of the isotopic and trace element measurements. Because of this formulation order of
120 magnitude fluctuations in lake volume cannot be modeled by this approach. Fundamentally, this
121 model quantifies the observations made by previous studies that qualitatively employed end-
122 member mixing (from a fresh source to an evaporative lake) in closed-basin lacustrine deposits
123 based on the covariance of Sr/Ca, Mg/Ca, $\delta^{18}\text{O}$ and $\delta^{13}\text{C}$ (for example, M ller and others, 1972;
124 Eugster and Kelts, 1983; Talbot, 1990; Li and Ku, 1997; Garnett and others, 2004; Davis and
125 others, 2009; Horton and Oze, 2012; McGee and others, 2012; Chamberlain and others, 2013;

126 Horton and others, 2015). We do not incorporate variations in $\delta^{13}\text{C}$ in this initial iteration of
127 HyBIM; however, evaporative processes and lake residence times should also control the
128 systematics of the $\delta^{13}\text{C}$ of carbonates from terminal lake systems (see discussion in Horton and
129 others, 2015).

130 First, we establish the modeling framework using a system of total differential equations.
131 Second, we describe the Monte Carlo routine used to account for parameter and input data
132 uncertainty (for example, Fantle, 2010; Royer and others, 2014). Third, we discuss the input
133 dataset (the time series of measurements) and necessary input parameters. Finally, we describe
134 the quantification of the partial derivatives necessary to constrain the model and necessary input
135 parameters. This model is available as a generic R code built for input of data from any time
136 series of biogenic carbonate from the authors website (<http://paleoclimate.stanford.edu>). For
137 illustrative purposes, we apply HyBIM to two ostracod valve datasets covering different
138 timescales: (1) the Cretaceous Songliao Basin, northeast China, and (2) Holocene Lake
139 Miragoane, Haiti. All model parameters are summarized in table 1 and a schematic of the model
140 structure is presented in figure A1.

141 *Model Framework*

142 Here, we present a modeling framework that produces a time series of temperature
143 changes, effects of evaporation, and relative volume estimates for runoff for carbonate-bearing
144 (here ostracods) paleolake records. Chivas and others (1986a) previously suggested a
145 quantitative framework by which a unique solution for paleotemperature and paleosalinity could
146 be calculated using paired Mg/Ca and $\delta^{18}\text{O}$ measurements. Following this observation, we write
147 three total differential equations for lake water that describe the effects of temperature,
148 evaporation, and runoff/precipitation on the oxygen isotopic and trace element concentration of

149 ostracods in a hydrologically closed lake. The three total differential equations (for lake water
 150 $\delta^{18}\text{O}$, [Mg], and [Sr]) are:

$$151 \quad d(\delta^{18}\text{O}) = \left(\frac{\partial(\delta^{18}\text{O})}{\partial T} \right) dT + \left(\frac{\partial(\delta^{18}\text{O})}{\partial F_{\text{evap}}} \right) dF_{\text{evap}} + \left(\frac{\partial(\delta^{18}\text{O})}{\partial F_{\text{input}}} \right) dF_{\text{input}} \quad (1)$$

$$152 \quad d[\text{Sr}] = \left(\frac{\partial[\text{Sr}]}{\partial T} \right) dT + \left(\frac{\partial[\text{Sr}]}{\partial F_{\text{evap}}} \right) dF_{\text{evap}} + \left(\frac{\partial[\text{Sr}]}{\partial F_{\text{input}}} \right) dF_{\text{input}} \quad (2)$$

$$153 \quad d[\text{Mg}] = \left(\frac{\partial[\text{Mg}]}{\partial T} \right) dT + \left(\frac{\partial[\text{Mg}]}{\partial F_{\text{evap}}} \right) dF_{\text{evap}} + \left(\frac{\partial[\text{Mg}]}{\partial F_{\text{input}}} \right) dF_{\text{input}} \quad (3)$$

154 where $\delta^{18}\text{O}$ is the oxygen isotopic composition of the lake water determined from
 155 biogenic carbonate measurements corrected for species-specific vital effects, [Mg] and [Sr] are
 156 the lake water concentrations of Mg^{2+} and Sr^{2+} determined from the Sr/Ca and Mg/Ca ratios
 157 measured in the biogenic carbonate, T is mean annual surface air temperature (K) for the lake
 158 basin, F_{evap} is the fraction of the lake evaporation, and F_{input} is the fractional lake volume
 159 increase due to changes in runoff and precipitation (see table 1).

160 We treat equations 1-3 as a system of total differential equations that can be solved for
 161 each time step of the first derivative of the [Mg], [Sr], and $\delta^{18}\text{O}$ time series (that is, $x = \mathbf{A}^{-1}\mathbf{b}$,
 162 where matrix \mathbf{A} is composed of the partial derivatives, the \mathbf{b} vector is the first derivative of the
 163 input dataset (left side of eqs 1 to 3) and x is the solution vector of $(dT, dF_{\text{evap}}, \text{ and } dF_{\text{input}})$). We
 164 do so by determining the partial derivatives for a specific lake system, calibrated using modern
 165 watershed/lake chemistry data and knowledge of the specific ostracod species. Interpolation to
 166 an evenly spaced time series is required, which we accomplish using an Epanechnikov kernel
 167 smoother applied to the input data. We assume that within each time step, lake evaporation
 168 and/or lake volume change does not change more than 20%, and we approximate all derivatives
 169 according to this assumption (that is at 10%). The model output is a time series of the solution

170 vector (dT , dF_{evap} , and dF_{input}). dF_{evap} and dF_{input} are combined to give the fractional net volume
171 increase for each time-step (see fig. A1). We use a Monte Carlo approach to account for
172 uncertainty in the input parameters and in the input dataset, which we derive from kernel
173 smoothing.

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175 *Monte Carlo routine for uncertainty quantification*

176 Given the assumptions that underlie the input parameters and data set for this model it is
177 critical to quantitatively assess the errors associated with the calculated runoff input, temperature
178 changes, and evaporative effects. Thus, we use a Monte Carlo routine to account for two types
179 of uncertainty. The first is uncertainty in the input dataset. Since most paleoclimate records
180 display uneven variance and non-uniform sampling density, it is necessary to account for this by
181 producing datasets for each iteration based on the statistics (time series of the mean and
182 residuals) derived from kernel smoothing of the dataset (see below). To do so, for each Monte
183 Carlo iteration we implement a bootstrapping method whereby we account for input dataset
184 uncertainty by re-sampling residuals. The second type of uncertainty accounted for by our model
185 is the uncertainty in the input parameters. The input parameters are best determined by modern
186 watershed and lake chemistry (when available) and knowledge of the species precipitating the
187 biogenic carbonate (described below). Within each Monte Carlo iteration, we derive a time series
188 of partial derivatives based on the input parameters. Input parameter uncertainty distributions are
189 assumed to be normal distributions, requiring that uncertainty is quantified by as many modern
190 measurements of watershed chemistry as possible. The partial derivatives are substituted into the
191 \mathbf{A} matrix at each time step.

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Input dataset requirements and interpolation

There are two requirements for the input dataset that need to be met for this model. First, the modeled Mg/Ca, Sr/Ca, and $\delta^{18}\text{O}$ time series must be of sufficient resolution to resolve climatic events of interest and the time step must be greater than the residence time of these elements in a lake. Thus, in order to use the dataset in the system of equations (left side of eqs 1 to 3), the time series must be interpolated to even time steps, requiring a sufficiently resolved age model for the Mg/Ca, Sr/Ca, and $\delta^{18}\text{O}$ measurements. Smoothing of each time series (Mg/Ca, Sr/Ca, and $\delta^{18}\text{O}$) is performed using an Epanechnikov kernel and interpolated to an even time step following a data driven least squares cross-validation to select the appropriate kernel bandwidth (Hayfield and Racine, 2008). The Epanechnikov kernel (Epanechnikov, 1969) is used because it has finite boundaries (instead of Gaussian kernel) and is smooth (compared to a triangle or uniform kernel) (see Fan, 1992; Danese and others, 2014). Kernel smoothing of the time series is implemented using the ‘np’ package in R (Hayfield and Racine, 2008). The additional advantage of using a kernel smoother is that uncertainty of the interpolated dataset can be quantified along the time series (mean and residuals) and input into the Monte Carlo routine.

While high-resolution interpolation of the smoothed dataset is desirable to resolve climatic events of interest, linear interpolation of the input dataset to an even time step (Δt) must be such that $\Delta t \gg \tau_{\text{res}}$, where τ_{res} is the residence time (inferred from lake geometry and average input or evaporative fluxes, for example Gibson and others, 2002; Jasechko and others, 2014). For lakes with no modern analogue (see Cretaceous Songliao Basin example), first-order estimates for τ_{res} can be approximated using scaling relationships between outcrop size and basin geometry (Hendriks and others, 2012), which in combination with facies identification can be used to determine estimates of the relationship between potential accommodation and basin

216 average precipitation/evaporation (Carroll and Bohacs, 1999). Thus, due to the formulation and
217 assumptions of the mixing and mass conservation relationships derived below, resolving
218 hydrologic or climatic events over intervals equal to or shorter than τ_{res} is not possible within this
219 modeling framework. This implies that, given the ‘water equivalency rule’ for a region of
220 interest (Hendriks and others, 2012), paleoclimate records from small lake systems, which
221 integrate smaller watersheds and have shorter residence times, provide the highest fidelity
222 temporal records of hydrologic cycle changes. Furthermore, determination of the lake
223 hypsometry and/or outcrop extent (for example, Reheis 1999; Sack, 2009; Steinman and others,
224 2013; Smith and others, 2014; Doebbert and others, 2014) ensures that the modeling assumptions
225 outlined above are met.

226 The second requirement for the model is that all of the input data need to be placed in
227 terms of lake composition. Although we use measured values of Mg/Ca, Sr/Ca, and $\delta^{18}\text{O}$ of
228 ostracods, these values need to be corrected so that they represent the values of these elements
229 and isotopes in the lake water. To make this correction one must correct for “vital effects” and
230 temperature. Correcting for vital effects is relatively straightforward as the measured vital effect
231 is simply subtracted from the measured ostracod values. Vital effects associated with the
232 calcification of biogenic carbonate are observed because shell carbonate is not precipitated in
233 isotopic equilibrium with water (Holmes and Chives, 2002). Vital effects observed in ostracod
234 $\delta^{18}\text{O}$ are positive (0.3 to 2.5 ‰) and have been observed to be constant within individual genera
235 (Xia and others, 1997a,b; von Grafenstein and others, 1999; Chivas and others, 2002; Didie and
236 Bauch, 2002). Since vital effects are not temperature-dependent, data from a variety of different
237 modern species fall on slopes close to the inorganic calcite equilibrium slope (-0.250 ‰/K) of
238 Kim and O’Neill (1997) (see compilation by Marco-Barab and others, 2012). Our model ideally

239 should be used with a time series produced by a single ostracod species or genera. Although, if
240 multiple species are measured (for example, Lister and others, 1991) this could be accounted for
241 using vital effect offsets.

242 In contrast, correcting for temperature effects is less straightforward and could, if done
243 incorrectly, lead to “circular reasoning” since we are attempting to constrain temperature
244 changes in the model. We assume temperature could vary from 10 to 35 °C (uniform
245 distribution). For each Monte Carlo iteration we select a starting temperature and assume that
246 $\delta^{18}\text{O}$ of the lake water is in equilibrium with the measured $\delta^{18}\text{O}$ of ostracods using the
247 temperature-dependent fractionation relationship of Kim and O’Neill (1997) corrected for vital
248 effects. We avoid “circular reasoning” since our system of linear equations calculates the relative
249 changes in temperature, dT (in the x vector), using the first derivative of the $\delta^{18}\text{O}$ of the lake
250 water (in the b vector), not the absolute temperature.

251 Distribution coefficients (K_D -values) relating trace element to calcium ratios are
252 commonly determined for biogenic carbonates through modern and/or culturing studies. The
253 distribution (or partition) coefficient is defined as:

$$254 \quad K_D[\text{M}] = \frac{\text{M} / \text{Ca}_{\text{water}}}{\text{M} / \text{Ca}_{\text{shell}}} \quad (4)$$

255 where M is the trace metal, such as Sr, Mg, or U, and M/Ca are molar ratios. K_D -values for Mg
256 and Sr are both less than one, meaning that both trace metals are actively excluded during
257 calcification. Additionally, Chivas and others (1986b) demonstrated that K_D -values are similar
258 among members of the same or closely related genera.

259 In many species, K_D has been shown to be temperature-dependent. In most ostracod
260 species, there is little or no temperature effect on Sr/Ca (Chivas and others, 1986; Holmes and
261 Chivas, 2002, Marco-Barab and others, 2012), but the Mg/Ca K_D in ostracods is temperature-

262 dependent (Engstrom and Nelson, 1991; DeDeckker and others, 1999; Holmes and Chivas,
263 2002). For the example datasets used in this paper, we use species-specific K_D -values (or from
264 related genera when not available), and uncertainties are obtained from regression statistics of
265 the original datasets (table 2). To place the input data [Mg] and [Sr] in terms of lake composition
266 (b vector) we calculate the Mg/Ca K_D (and Sr/Ca K_D if necessary) using the temperature and lake
267 water [Ca] selected for each Monte Carlo iteration.

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Determining Partial Derivatives

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In the following sections each of the partial derivatives are derived or determined using

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either mass conservation (for example, $\frac{\partial[\text{Mg}]}{\partial F_{\text{evap}}}$) and mixing (for example, $\frac{\partial[\text{Mg}]}{\partial F_{\text{vol}}}$), or empirical

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relationships from environmental and/or laboratory measurements (for example, $\frac{\partial(\delta^{18}\text{O})}{\partial T}$).

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Temperature Partial Derivatives

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To solve for the oxygen isotope partial derivative $\frac{\partial(\delta^{18}\text{O})}{\partial T}$ requires knowing how $\delta^{18}\text{O}$ of

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meteoric water (precipitation and runoff) varies as a function of temperature. We recognize that

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there are numerous factors affecting the $\delta^{18}\text{O}$ of precipitation beyond that of temperature, which

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include seasonality, vapor recycling, moisture source et cetera. However, the commonly held

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assumption that underpins terrestrial paleoclimate studies is the well-known positive correlation

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between $\delta^{18}\text{O}$ values of precipitation and temperature for temperate and high latitude areas

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(Dansgaard, 1964). For the mid-latitude site (Songliao Basin) we use the observed relationship

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between temperature and precipitation Rozanski and others (1993) of 0.58 ‰/K, as has been

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used in numerous studies to calculate the temperature for paleoclimate archives in mid- to high-

283 latitude sites, such as paleosols (for example, Koch and others, 2003), paleolakes (for example,
284 Anderson and others, 2001), and ice cores (see Jouzel and others, 1997 and references therein).
285 For the low latitude site (Lake Miragoane, Haiti) it is unlikely that the correlations of Rozanski
286 and others (1993) apply as these are for mid- to high-latitudes. Although it is not ideal to use the
287 approach we outline in this paper to low latitudes because temperature is not as well correlated to
288 the $\delta^{18}\text{O}$ of precipitation, we use this site only as an example of how this approach can be used in
289 lakes because this record offers the type of data that are necessary for these calculations.
290 Recognizing these limitations we use a slope of 0.26‰/K for the tropical sites (see fig. A2). For
291 both cases we incorporate the error associated with the empirical temperature vs. $\delta^{18}\text{O}$
292 correlation in the Monte Carlo.

293 In our model, thus, one of the assumptions inherent in our calculations is that temperature
294 is the primary driver of $\delta^{18}\text{O}$ value of water input to the lake. Note that since the slope between
295 temperature and $\delta^{18}\text{O}$ of precipitation can and does vary geographically, more accurate
296 approaches can be tailored for individual sites by measurements of site-specific correlations
297 between temperature and $\delta^{18}\text{O}$ of precipitation.

298 In addition, to the partial $\frac{\partial(\delta^{18}\text{O})}{\partial T}$ discussed above it is necessary to place the ostracod
299 values as the $\delta^{18}\text{O}$ of lake water for these calculations (b vector of eqs 1 to 3). To do this we need
300 to account for both vital effects and the temperature-dependent isotopic fractionation (see above).

301 In addition, there are minor temperature effects on the Sr/Ca (typically none) and Mg/Ca
302 (see above discussion). Since the inputs (b vector of eqs 1 to 3) are placed in terms of lake
303 composition, after accounting for the Mg/Ca or Sr/Ca of the lake water and selected temperature

304 for the Monte Carlo iteration the temperature partial derivatives ($\frac{\partial[\text{Mg}]}{\partial T}$ and $\frac{\partial[\text{Sr}]}{\partial T}$) are equal to
305 zero.

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307 *Evaporation Partial Derivatives*

308 To account for the evaporative concentration of trace elements, we assume mass
309 conservation of Sr and Mg. Thus, this model is not applicable to brine or saline environments
310 (see Jones and others, 1977; Eugster and Jones, 1979) nor is it applicable to systems that form
311 large deposits of chemical sediments with high Mg and/or Sr concentrations. For biogenic
312 carbonates, we apply the applicable distribution coefficient (K_D) and take the first derivative. In
313 doing so, we assume that the Sr/Ca and Mg/Ca measured in the biogenic carbonates are faithfully
314 recording changes in the Sr and Mg concentrations of the lake water. Assuming mass
315 conservation, the change in solute M concentration (from the initial concentration to an increased
316 concentration at time 2) during fractional lake evaporation (F_{evap} , fraction remaining, from 0 to 1,
317 where 1 is fully evaporated) is given by the equation (fig. 1):

$$318 \quad [M]_2 = \frac{[M]_{\text{initial}}}{(1 - F_{\text{evap}})} \quad (5)$$

319 Solving for the partial derivative of equation 5 has the analytical solution:

$$320 \quad \frac{\partial[M]}{\partial F_{\text{evap}}} = \frac{[M]_{\text{initial}}}{(1 - F_{\text{evap}})^2} \quad (6)$$

321 This relationship is non-linear; thus, to provide a linear slope for $\frac{\partial[M]}{\partial F_{\text{evap}}}$ we assume that for any
322 given time step, the lake does not evaporate more than 20% by volume. By inspection of
323 equation 6, the average evaporation between 0 to 20%, given by $F_{\text{evap}} = 0.1$, yields a slope of

324 $\frac{[M]_{\text{initial}}}{(0.9)^2}$. Therefore, the initial trace element concentration (that is, the Mg and Sr
325 concentrations), which we assume to be approximated using the observed distribution of trace
326 element measurements, is important for setting $[M]_{\text{initial}}$ at each time step.

327 The evaporative enrichment of lake water $\delta^{18}\text{O}$ with progressive evaporation was
328 originally parameterized by Craig and Gordon (1965). The limitation of applying the Craig and
329 Gordon (1965) evaporation model to lacustrine paleoclimate records, as outlined in detail by
330 Gonfiantini (1986), is the large number of input parameters and the difficulty in constraining the
331 isotopic composition of the evaporated water vapor (see discussion in Jones and Imbers, 2010).
332 Recent work has attempted to simplify evaporative assumptions (Benson and White, 1994; Jones
333 and others, 2007; Jones and Imbers, 2010; Placzek and others, 2011), but numerous input
334 parameters are still required, making the generic application of these lake water evaporation
335 models to paleoclimate records challenging.

336 Central to the difficulties encountered by previous researchers is the influence of
337 humidity on the evolution of the isotopic composition of an evaporating water body (Gonfiantini,
338 1986). This is due to changes in the kinetic enrichment factor due to changes in humidity (Gat,
339 1970; Merlivat, 1978; Merlivat and Jouzel, 1979). However, if within a given time step lake
340 evaporation does not exceed ~25% total lake volume and humidity is <90%, the isotopic
341 evolution of an evaporating water body can be approximated by a Rayleigh relationship
342 (Gonfiantini, 1986). Thus, we derive the partial derivative for $\delta^{18}\text{O}$ and fractional lake
343 evaporation as the first derivative of the Rayleigh equation (fig. 1):

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$$\frac{\partial(\delta^{18}\text{O})}{\partial F_{\text{evap}}} = (\alpha - 1)(\delta^{18}\text{O}_1 + 1000)(1 - F_{\text{evap}})^{(\alpha-2)} \quad (7)$$

345 where α is the combined fractionation factor of the temperature-dependent equilibrium
346 fractionation factor (Horita and Weslowski, 1996) and humidity-dependent kinetic fractionation
347 factor (Gonfiantini, 1986), F_{evap} is the fraction of the lake evaporation (as above) and $\delta^{18}\text{O}_{\text{initial}}$ is
348 the initial isotopic composition of the lake from the measured $\delta^{18}\text{O}$ of the biogenic carbonate
349 corrected for vital effects (see below). While a simplification of evaporative processes, assuming
350 a Rayleigh relationship and a combined fractionation factor in this manner has successfully been
351 applied to both surface soil reservoir and lake system modeling (for example, Chamberlain and
352 others, 2014; Caves and others, 2015). We assume that relative humidity for each Monte Carlo
353 iteration can vary from 50 to 90 % (uniform distribution), and temperature varies from 5 to 35 °C
354 (uniform distribution) as determined for each iteration (as described above). By doing so we
355 calculate the combined fractionation factor, α , using the equations of Horita and Weslowski
356 (1996) and Gonfiantini (1986) (see fig. 1). The humidity and temperature ranges selected here
357 are conservative and broadly apply to both illustrative lake systems used in the examples below.
358 The relevant latitude and geographic setting of the lake system being modeled should inform the
359 humidity and temperature ranges chosen as model input.

360

361 *Lake Input Partial Derivatives*

362 Determination of the lake input partial derivatives is similar for both trace elements and
363 oxygen isotopes. We rely on binary mixing equations assuming that the isotopic and chemical
364 composition of water entering the lake is sufficiently well characterized and relatively invariant
365 (relative to the lake water). Water in terminal lakes is sufficiently evaporatively enriched relative
366 to the input $\delta^{18}\text{O}$ that in most examples, the input water $\delta^{18}\text{O}$ composition is typically statistically
367 distinguishable from the lake water $\delta^{18}\text{O}$ composition (see for example compilation by Horton

368 and Oze, 2012). This is similar for trace elements in terminal lake systems, such that the input
369 concentration of Sr and Mg in terminal lakes is typically more dilute than the lake water.

370 Given these principles, we define the partial derivative relating increased lake volume,
371 from the addition of source water (F_{input} , which varies from 1 to infinity, where 1 is the original
372 lake volume) and variations in $\delta^{18}\text{O}$ as the first derivative of a binary mixing relationship (fig. 2):

$$373 \quad \frac{\partial(\delta^{18}\text{O})}{\partial F_{input}} = \frac{(\delta^{18}\text{O})_{source} - (\delta^{18}\text{O})_{initial}}{(F_{evap})^2} \quad (8)$$

374 where $\delta^{18}\text{O}_{source}$ is the meteoric water composition and $\delta^{18}\text{O}_{initial}$ is determined as previously
375 described. The meteoric water $\delta^{18}\text{O}$ composition should be determined by direct observation, by
376 upstream fluvial carbonates (for example Ibarra and others, 2015) or by assuming an empirical
377 relationship related to the amount of annual rainfall (amount effect), as observed in many
378 tropical systems (Risi and others, 2008). Similarly for trace element concentrations:

$$379 \quad \frac{\partial[M]}{\partial F_{input}} = \frac{[M]_{source} - [M]_{initial}}{(F_{evap})^2} \quad (9)$$

380 where M is the Sr or Mg concentration, $[M]_{source}$ refers to the runoff water concentrations, and
381 $[M]_{initial}$ is determined as previously described from the measured Mg/Ca and Sr/Ca of the
382 biogenic carbonate.

383

384 *Input parameter requirements*

385 There are several input parameter requirements that need to be satisfied for robust use of
386 this model. First, measurements of solute chemistry ([Sr], [Mg], and [Ca] from lake water and/or
387 runoff) and $\delta^{18}\text{O}$ of meteoric water are necessary to constrain the mixing equation end-members.
388 This can best be done by measuring the elemental and isotopic composition of modern rivers and
389 precipitation in the lake to be studied or the site of the ancient lake as is done here in the

390 Songliao Basin (table 2). There are obvious complications to this approach since the drainage
391 basin may have changed through time as well as the isotopic composition of precipitation – for
392 example by a change in moisture source. In addition, the uncertainty (standard deviation) of the
393 end-members is required. This can be quantified through repeat measurements of stream
394 water/subsurface runoff chemistry.

395 Second, empirical relationships for temperature effects on the species-specific partition
396 coefficient (for Mg/Ca) are required; such as those fit by Engstrom and Nelson (1991) and
397 DeDecker and others (1999). As discussed above, species-specific vital effects for $\delta^{18}\text{O}$ offsets
398 are applied uniformly prior to derivation of the partial derivatives from the mixing and mass
399 conservation equations. Input parameters are supplied to HyBIM as the mean and standard
400 deviation, assuming a normal distribution. However, implementation of other probability
401 distributions (such as uniform distributions) is possible. The probable temperature and relative
402 humidity ranges (used for the $\delta^{18}\text{O}$ equilibrium fractionation equations and Mg/Ca K_D values),
403 which are treated as uniform distributions, are specified by the user and should be informed by
404 paleoenvironmental, latitudinal, climate modeling, and/or modern observations.

405

406

EXAMPLE APPLICATIONS

407 We apply HyBIM to two lacustrine paleoclimate records covering differing timescales,
408 geochemical conditions, ostracod species, and dataset resolutions (figs. 3 and 4). We chose these
409 two data sets because: (1) they had the elemental and isotopic measurements necessary for using
410 this model and; (2) they represent two very different cases that demonstrate the utility and
411 flexibility and limitations of the HyBIM for a variety of biogenic carbonate paleoclimate records.
412 In each case, the original age model is used for all datasets and input parameters are constrained

413 using modern catchment and lake chemistry and species-specific partition coefficient calibrations.
414 Sampling resolution, the least squares cross-validated kernel bandwidths, length of the
415 paleoclimate record, and input parameter sources are listed in table 2.

416

417 *Lake Miragoane, Haiti (Hodell and others, 1991; Curtis and Hodell, 1993)*

418 The paleoclimate records from Holocene Lake Miragoane in Haiti (Hodell and others,
419 1991; Curtis and Hodell, 1993; Higuera-Gundy, 1999) were one of the first to use detailed, high-
420 resolution stable isotope and trace element measurements on lacustrine ostracods. This
421 hydrologically closed lake provides a complete record of the Holocene at high resolution (see
422 age resolutions for $\delta^{18}\text{O}$, Mg/Ca and Sr/Ca records in table 2). Two cores were recovered and
423 sampled at fine (~10 cm) resolution for $\delta^{18}\text{O}$ and coarser (~150 cm) resolution for Mg/Ca and
424 Sr/Ca (Curtis and Hodell, 1993). The discrepancy in sample resolution results in the cross-
425 validated kernel bandwidth for $\delta^{18}\text{O}$ (bandwidth = 39 years) to be much shorter than the Mg/Ca
426 and Sr/Ca records (422 and 440 years, respectively) (fig. 3A). Data from both cores were
427 combined and kernel smoothed using the original age model.

428 The elemental and isotopic data for these studies were from ostracods identified as
429 *Candona* sp., by R. Forester (see discussion in Curtis and Hodell, 1993), which is an ostracod
430 species closely related to *Candona rawsoni*. See table 2 for detailed model input parameters,
431 including the partition coefficients for *Candona rawsoni* as determined by Engstrom and Nelson
432 (1991).

433 The modeled temperature and lake volume changes for the Lake Miragoane record are
434 largely in accordance with the expected response (see interpretation in Curtis and Hodell, 1993,
435 their fig. 8). These authors suggested based on the isotopic and elemental data that lake levels

436 were highest and climate was “mesic” (wetter and hotter) during the early Holocene, peaking
437 between 7,000 and 4,000 years BP (Hodell and others, 1991; Curtis and Hodell, 1993). In the late
438 Holocene they suggest that between ~4,000 and ~2,500 years BP there was a two-step increase in
439 aridity towards lower lake level and increased salinity, based primarily on the oxygen isotopes
440 (Hodell and others, 1991), followed by wetter conditions beginning at ~1,000 year BP based on
441 additional evidence from the trace element measurements (Curtis and Hodell, 1993).

442 Our model agrees with this interpretation and shows that modeled temperature and lake
443 volume covary. Lake volume and temperature increase to a peak at ~6300 years BP, decline to a
444 minimum at ~2000 years BP, and increase again nearing present day. The deglacial warming
445 (~10,000 to 7,000 years BP), and increasing aridity (from ~4,000 to 1,000 years BP) are captured
446 by the predicted temperature fluctuations. Driven by the covariation in the input datasets, the

447 modeled temperature is substantially different than that expected from just using the $\frac{\partial(\delta^{18}\text{O})}{\partial T}$
448 empirical relationship of 0.26 ‰/°C (red line of fig. 3B; relationship derived in fig. A2). In
449 addition, while the higher resolution $\delta^{18}\text{O}$ record determines the sub-1000-year variations in
450 temperature, the long-term trends largely reflect the trace element records. The sampling
451 resolution discrepancy of the trace elements (low resolution) and $\delta^{18}\text{O}$ records (high resolution)
452 is not necessarily ideal, but our results demonstrate that, by kernel smoothing the records and
453 interpolating to even time-steps, the problem of differing sampling resolution can be resolved.

454

455 *Songliao Basin, China (Chamberlain and others, 2013)*

456 The Songliao Basin is a Cretaceous terrestrial lake basin that contains up to 10,000 m of
457 fluvial-lacustrine, volcanoclastic and alluvial sediments (Feng and others, 2010; Wang and others,
458 2013). During the first phase (SK-1) of the International Continental Scientific Drilling Project’s

459 (ICDP) efforts to recover strata covering the entire Cretaceous, a total of 2,486 m of core were
460 recovered that span the late Turonian to the end Cretaceous (Wan and others, 2013; Deng and
461 others, 2013; Wu and others, 2014). Recent paleoclimate reconstruction efforts have used a
462 variety of proxies, including ostracods from lacustrine facies (Chamberlain and others, 2013) and
463 paleosol carbonate nodules (Huang and others, 2013; Gao and others, 2015). We model the
464 Sr/Ca, Mg/Ca and $\delta^{18}\text{O}$ ostracod record originally published by Chamberlain and others (2013)
465 spanning 84-88 Ma (fig. 4A). Data is kernel smoothed on the original age model (Wan and
466 others, 2013; Wang and others, 2013; Chamberlain and others, 2013), and this portion of the
467 record was selected because of the high density sampling through this period, relatively stable
468 source area (based on $^{87}\text{Sr}/^{86}\text{Sr}$), and the likely existence of Ocean Anoxic Event 3 (OAE 3 at
469 ~85.5 Ma; Waple, 2012). Because the ostracod genus *Cypridea* sampled by Chamberlain and
470 others (2013) is extinct, we use partition coefficient and vital effect calibrations for the extant
471 genus *Cyprideis*, a closely related genus also of the *Cyprididae* family (table 2). See table 2 for
472 detailed model input parameters.

473 The relatively invariant (kernel smoothed) Mg/Ca and Sr/Ca records (fig. 4A) result in
474 several interesting observations when HyBIM is applied to the Songliao Basin ostracod record.
475 The Mg/Ca and Sr/Ca records demonstrate much greater spread around the mean kernel-
476 smoothed values and, due to slightly lower sampling density, have a greater cross-validated
477 kernel bandwidth than the $\delta^{18}\text{O}$ record (62 kyrs vs. 241 kyrs and 219 kyrs; fig. 4A). Because of
478 the relatively invariant Mg/Ca and Sr/Ca record, the modeled temperature is similar to the result
479 expected if a $\frac{\partial(\delta^{18}\text{O})}{\partial T}$ empirical relationship of 0.58 ‰/°C is applied to the kernel smoothed
480 mean of the $\delta^{18}\text{O}$ record (red line in fig. 4B), unlike the Lake Miragoane record.

481 We applied the HyBIM to a portion of the Songliao record given in Chamberlain and
482 others (2013) from 88 to 84 Ma because this time interval captures a portion of the Oceanic
483 Anoxic Event 3 (OAE 3) during a time of global warming. Moreover, we have excellent oxygen
484 and trace element data for this time range in the Songliao Basin. It is recognized that unlike
485 earlier OAEs, OAE 3, may be a series of events distributed over longer time frames and is
486 recorded predominantly in the western hemisphere (Wagreich, 2012). Thus, we are interested in
487 how the temperature record in the Songlia Basin recorded this “event”. Our results show peaks
488 of warming of $\sim 6^{\circ}\text{C}$ between 86 and 85 Ma and again between 85 and 84 Ma. These two warm
489 periods are consistent with multiple events defining OAE 3, but cannot not be correlated with
490 those in marine sections because: 1) the age constraints in the Songlia Basin lack the necessary
491 time resolution; and 2) there are multiple carbon isotope excursions during OAE 3 that vary both
492 temporally and spatially across the globe (Wagreich, 2012). Nevertheless, our results do show
493 multiple warming events during this time interval of OAE 3. In addition, the HyBIM results
494 agree with the interpretation of increasing lake size, based on outcrop extent, during this time
495 interval (Feng and others, 2010), suggesting that over this interval lake volume increased by
496 $\sim 10\%$. However, we point out that due to the large spread in the measured Sr/Ca and Mg/Ca, the
497 modeled volume changes are not particularly robust.

498

499

LIMITATIONS AND GUIDELINES

500

501

502

The modeling framework presented in this paper represents a new approach to
quantitatively constraining the hydrologic balance and temperature fluctuations as recorded by
the trace elements and stable isotopes of biogenic lacustrine carbonate. Inherently the modeling

503 of paleoclimate records requires simplifying assumptions. As such, we provide several
504 guidelines for assessing the potential application of HyBIM to a lake system:

505 (1) Lake systems with highly variable (inorganic) chemical sedimentation, typically driven
506 by order of magnitude changes in lake level, cannot be modeled using HyBIM. A
507 fundamental assumption of the evaporation partial derivatives is that we assume mass
508 conservation of the trace elements within each time step. In addition, we assume that
509 within each time step lake volume does not change by more than 10% (see derivation of
510 partial derivatives). Thus, HyBIM solutions should be limited to “balanced-filled” (Carroll
511 and Bohacs, 1999) lake systems with biogenic carbonate from periods of similar
512 lithologic deposition.

513 (2) Many large lakes break up into smaller lakes during desiccation due to complex
514 hypsometric basin geometries and watersheds (for example Quaternary Lake Lahontan;
515 Reheis and others, 2014). While this is not readily assessed from sediment cores alone,
516 we emphasize the need for determination of the lake hypsometry via shoreline and/or
517 outcrop extent (for example, Reheis, 1999; Sack, 2009; Zimmerman and others, 2011;
518 Steinman and others, 2013; Ibarra and others, 2014; Smith and others, 2014; Doebbert
519 and others, 2014). HyBIM should not be applied to these systems over intervals of
520 breakup, as the river chemistry of the smaller lake basins within a large system may differ
521 due to bedrock heterogeneity and catchment weathering processes.

522 (3) Well-constrained partition coefficients are necessary to place the measured Mg/Ca and
523 Sr/Ca (or other trace element measurements) in terms of lake water concentrations.
524 Presently modern studies of terrestrial biogenic carbonates from ostracods (for example,
525 Engstrom and Nelson, 1991; Xia and others, 1997a,b; Wansard and others, 1998; De

526 Deckker and others, 1999; Dettman and others, 2002; Holmes and Chivas, 2002; Dwyer
527 and others, 2002; Ito and Forester, 2009; Gouramanis and De Deckker, 2010; Marco-
528 Barba and others, 2012; Börner and others, 2013) represent some of the only calibrated
529 partition coefficients available for use in the HyBIM modeling framework outlined here.
530 Future application of this modeling framework to inorganic carbonate or other types of
531 biogenic carbonate from lake systems will require further measurement of trace elements
532 and calibration of partition coefficients.

533 (4) We assume that lake water temperature and the basin average air temperature are directly
534 proportional. HyBIM solves for temperature changes (ΔT), not absolute values of
535 temperature, but selects an absolute temperature for each Monte Carlo iteration used for
536 placing the measured Mg/Ca and $\delta^{18}\text{O}$ into lake water composition (see previous
537 discussion). For the lake systems with mean annual air temperature greater than 0 °C
538 included in a recent global lake temperature compilation the slope between the mean
539 annual water temperature and mean annual surface air temperature is indistinguishable
540 from 1 (slope = 1.02 ± 0.03 (1σ), $r^2 = 0.94$, $n = 81$, mean annual air temperatures from 0
541 to 27 °C; see dataset from Appendix A of Hren and Sheldon, 2012), suggesting that this
542 assumption of proportionality is valid.

543

544 CONCLUSIONS AND FUTURE MODEL REFINEMENT

545 In this paper, we develop and apply a new modeling framework using variations in $\delta^{18}\text{O}$
546 and trace elements (Mg and Sr) measured in biogenic lacustrine carbonates for closed basin
547 lacustrine paleoclimate records. By applying this modeling approach to two ostracod records, we
548 demonstrate the utility of HyBIM to quantify paleoenvironmental changes across different

549 timescales. Due to a lack of significant variation in the (kernel smoothed) Mg/Ca and Sr/Ca
550 records from the Songliao Basin, the $\delta^{18}\text{O}$ record primarily controls the predicted temperature
551 fluctuations and the volume changes are minimal. Additionally, the Lake Miragoane results
552 demonstrate how the combination of high-resolution and low-resolution datasets are accounted
553 for by HyBIM via kernel smoothing and interpolation to even time steps. Future application of
554 HyBIM to a high-resolution historical record from a small, constrained terminal lake system will
555 provide the best independent validation of this modeling methodology.

556 Two additions could provide further extensions to this modeling approach. First, over-
557 determination of the **A** matrix by adding a fourth equation to the system of equations describing
558 additional trace elements (such as U or Li; for example Holmes and others, 1995), δD (for
559 example Tierney and others, 2008; Feakins and others, 2014; Kirby and others, 2014) or $\delta^{13}\text{C}$
560 (controlled by similar processes described in Li and Ku, 1999; Horton and Oze, 2012; Horton
561 and others, 2015) would provide greater control on the partitioning of salinity changes due to
562 evaporation and dilution by volumetric increases. Second, additional isotope systems, such as Sr
563 or Pb isotopes, could be included as a fourth equation (the **A** matrix would be 4x4) and would
564 extend the function of HyBIM to also de-convolve other possible variables, such multiple
565 riverine inputs, rearrangement of the drainage basin, et cetera. For example, assuming different
566 watershed source regions have different Sr or Pb isotope signatures (and also trace element
567 concentrations and/or meteoric water $\delta^{18}\text{O}$ inputs), a fourth set of partial derivatives can be
568 derived to define the relationship between two distinct end-members. This approach could be
569 applied to the full Songliao Basin record (lower resolution) presented in Chamberlain and others
570 (2013), or to basins with sufficient data and known tectonic changes, such as Cenozoic basins in

571 the western United States (for example, Davis and others, 2009; Smith and others, 2014;
572 Doebbert and others, 2014).

573 The application of this modeling framework is not limited solely to lake systems. For
574 example, recently published speleothem records have measured $\delta^{18}\text{O}$, Mg/Ca, and Sr/Ca, in
575 addition to other trace elements (such as U/Ca, Ba/Ca) and isotope systems (such as ($^{234}\text{U}/^{238}\text{U}$)
576 and $^{87}\text{Sr}/^{86}\text{Sr}$) (for example, Oster and others, 2009; Steponaitis and others, 2015). By modifying
577 the modeling framework presented here the relative influence of temperature and vadose zone
578 residence times (influenced by prior carbonate precipitation) on the stable isotope and trace
579 element measurements could be quantitatively deconvolved. However, modern cave monitoring
580 studies to assess the variability and controls on the stable isotope and trace element variations in
581 cave drip water (for example, Fairchild and others, 2000; Musgrove and Banner, 2004; Wong
582 and others, 2011; Oster and others, 2012a), would be necessary for calibration. Similarly, trace
583 element and stable isotope measurements on pedogenic soil minerals and the associated soil pore
584 water in arid soil systems (for example Amundson and others, 1996; Oster and others, 2012b;
585 Maher and others, 2014) may provide an additional avenue for quantitative paleoclimate
586 reconstruction using a similar modeling framework.

587 Finally, the Monte Carlo approach presented in this paper only includes uncertainty in the
588 input parameters and input dataset. However, age-models in sedimentary settings, and many
589 terrestrial paleoclimate archives, including lakes, can be highly uncertain due to sedimentation
590 rate changes, hiatuses and a lack of dateable material (for example, Huybers and Wunsch, 2004;
591 Blaauw and Christen, 2011). Further extension of HyBIM to include incorporation of age model
592 uncertainty would provide added utility by including temporal uncertainty quantification of the
593 hydrologic response to climatic events and trends recorded by the lake carbonate geochemistry.

594 Recent work has included this type of Monte Carlo age model uncertainty into paleoclimate
595 reconstructions for individual records and large paleoclimate compilations (for example, Shakun
596 and others, 2012; Anchukaitis and Tierney, 2013; Tierney and others, 2013; Marcott and others,
597 2013; Steinman and others, 2014). Ultimately paleoclimate proxy modeling efforts, such as those
598 illustrated in this paper, are only valuable if the uncertainty of the timing and magnitude of
599 climatic changes is robustly quantified.

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- 1084

FIGURES

1085
1086 Figure 1. Illustration of evaporation relationships used to parameterize the partial derivatives.
1087 Inset plots show regions of linear approximation assuming $F_{\text{evap}} < 0.2$ within each time step (blue
1088 shading). Dashed lines are uncertainty. See text for equations describing relationships. (A)
1089 Rayleigh evaporation of $\delta^{18}\text{O}$, total (kinetic and equilibrium) fractionation, ϵ , is $13.5 + 4.7/-3.6\text{‰}$
1090 (5 to 35 °C and 50 to 90% humidity). (B) Mass conservation of solute, M (that is, Mg or Sr),
1091 with an initial lake concentration of 10 ± 2 mmol.

1092
1093 Figure 2. Illustration of mixing relationships used to parameterize the partial derivatives for
1094 volume increase. Inset plots show regions of linear approximation assuming $F_{\text{input}} < 1.2$ within
1095 each time step (blue shading). Dashed lines are uncertainty. See text for equations describing
1096 relationships. (A) $\delta^{18}\text{O}$ mixing (input water of $-15 \pm 2\text{‰}$, initial lake water of -3‰). (B) Mixing
1097 of initial concentration (10 ± 2 mmol) with a dilute input solute concentration of 3 mmol.

1098
1099 Figure 3. Illustrative Application of HyBIM to the Lake Miragoane Ostracod (*Candona* sp.)
1100 record. (A) Original $\delta^{18}\text{O}$, Mg/Ca and Sr/Ca records (grey dots) from Hodell and others (1991)
1101 and Curtis and Hodell (1993). Data are plotted on the original age model. For model input the
1102 data are kernel smoothed using an Epanechnikov kernel. The cross validated bandwidth (BW;
1103 see text for explanation) is listed for each record ($\delta^{18}\text{O}$, Mg/Ca and Sr/Ca). The solid black line is
1104 the mean and the dashed black lines are the 1σ . (B) HyBIM results for the Lake Miragoane
1105 records using partition coefficient and vital effect data from Engstrom and Nelson (1991) and
1106 Keatings (1999) derived for *Candona* sp. The red line is the empirical relationship for isotopes in

1107 precipitation (0.26‰/°C) derived from empirical tropical GNIP stations (fig. A2; after Rozanski
1108 and others, 1993).

1109

1110 Figure 4. Illustrative Application of HyBIM to the Songliao Basin Ostracod (*Cypridea* sp.)

1111 Record. (A) Original $\delta^{18}\text{O}$, Mg/Ca and Sr/Ca records (grey dots) from Chamberlain and others

1112 (2013). Data are plotted on the original age model of Wan and others (2013). For model input the

1113 data are kernel smoothed using an Epanechnikov kernel from 84 to 88 Ma (densely sampled

1114 portion of the record). The cross validated bandwidth (BW; see text for explanation) is listed for

1115 each record ($\delta^{18}\text{O}$, Mg/Ca and Sr/Ca). The solid black line is the mean and the dashed black lines

1116 are the 1σ . (B) HyBIM results for the Songliao Basin record using partition coefficient data from

1117 DeDeckker and others (1999) derived for *Cyprideis* sp., the extant, closely related genus of

1118 *Cypridea* sp. The solid line is the median and the dashed blue lines are the 95% confidence

1119 interval of the Monte Carlo estimation. The approximate position of OAE 3 is denoted by the red

1120 bar, which corresponds to a peak the predicted temperature. The red line is the empirical

1121 relationship of Rozanski and others (1993) for isotopes in precipitation (0.58 ‰/°C) derived

1122 from mid-latitude Global Network of Isotopes in Precipitation (GNIP) stations.

1123

1124 Figure A1. Schematic of HyBIM model structure. The model structure uses a matrix inversion to

1125 solve a system of three equations ($\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$) implemented at each time step to calculate changes

1126 in lake volume (from the combined evaporation and inputs) and basin average air temperature.

1127 After smoothing and interpolating to an even time series, the input dataset (time series of $\delta^{18}\text{O}$,

1128 Mg/Ca and Sr/Ca from biogenic carbonate), given a set of adjustable input parameters (right side

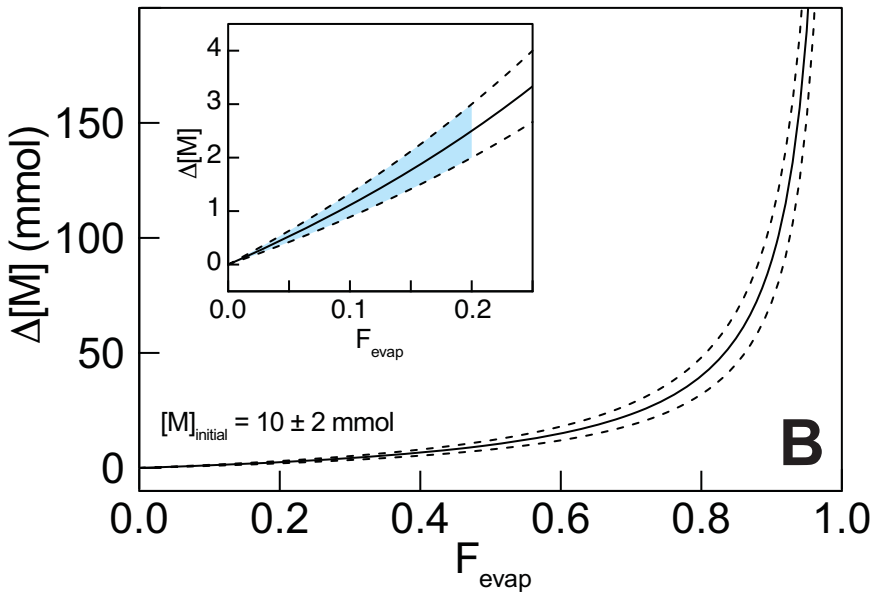
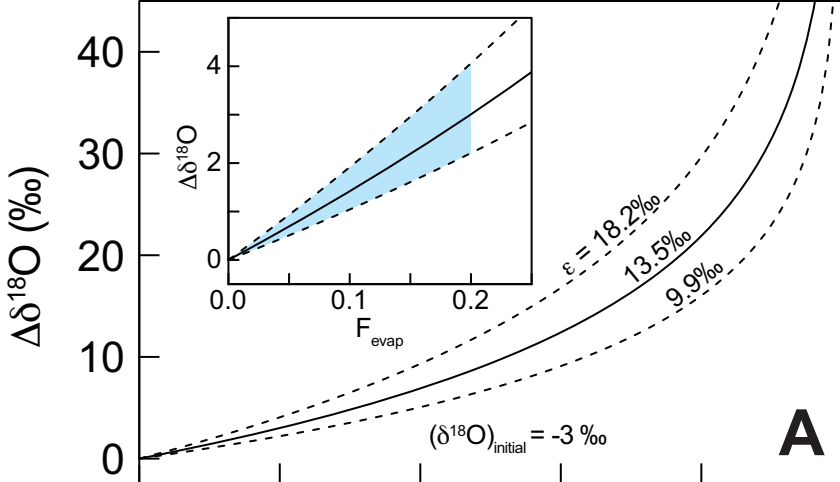
1129 of the fig.; table 1), is first placed in lake water composition ($\delta^{18}\text{O}$, [Mg] and [Sr] Lake Water).

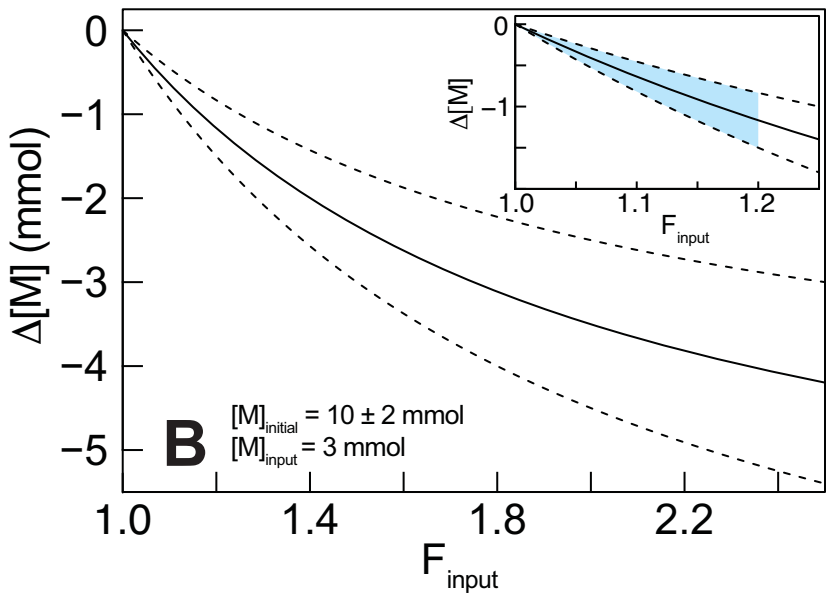
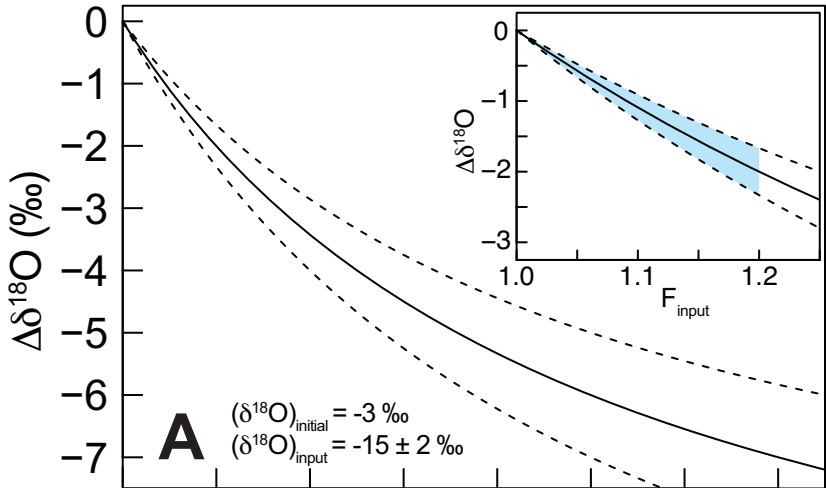
1130 The first derivative of the lake water time series is inputted as the \mathbf{b} vector at each time step
1131 ($d(\delta^{18}\text{O})$, $d[\text{Mg}]$ and $d[\text{Sr}]$). The partial derivatives that make up the \mathbf{A} matrix are substituted at
1132 each time step using mixing equations and evaporation equations (eqs 5 to 9 for F_{evap} and F_{input}
1133 derivatives), or estimated for temperature (the T derivatives) based on the geographic location
1134 (see text for details). For each Monte Carlo iteration the model produces a time series of the \mathbf{x}
1135 solution vector. To provide summary statistics after combining the evaporation and lake input
1136 variables to calculate changes in volume we calculate the median and 95% range (as in figs. 3
1137 and 4).

1138

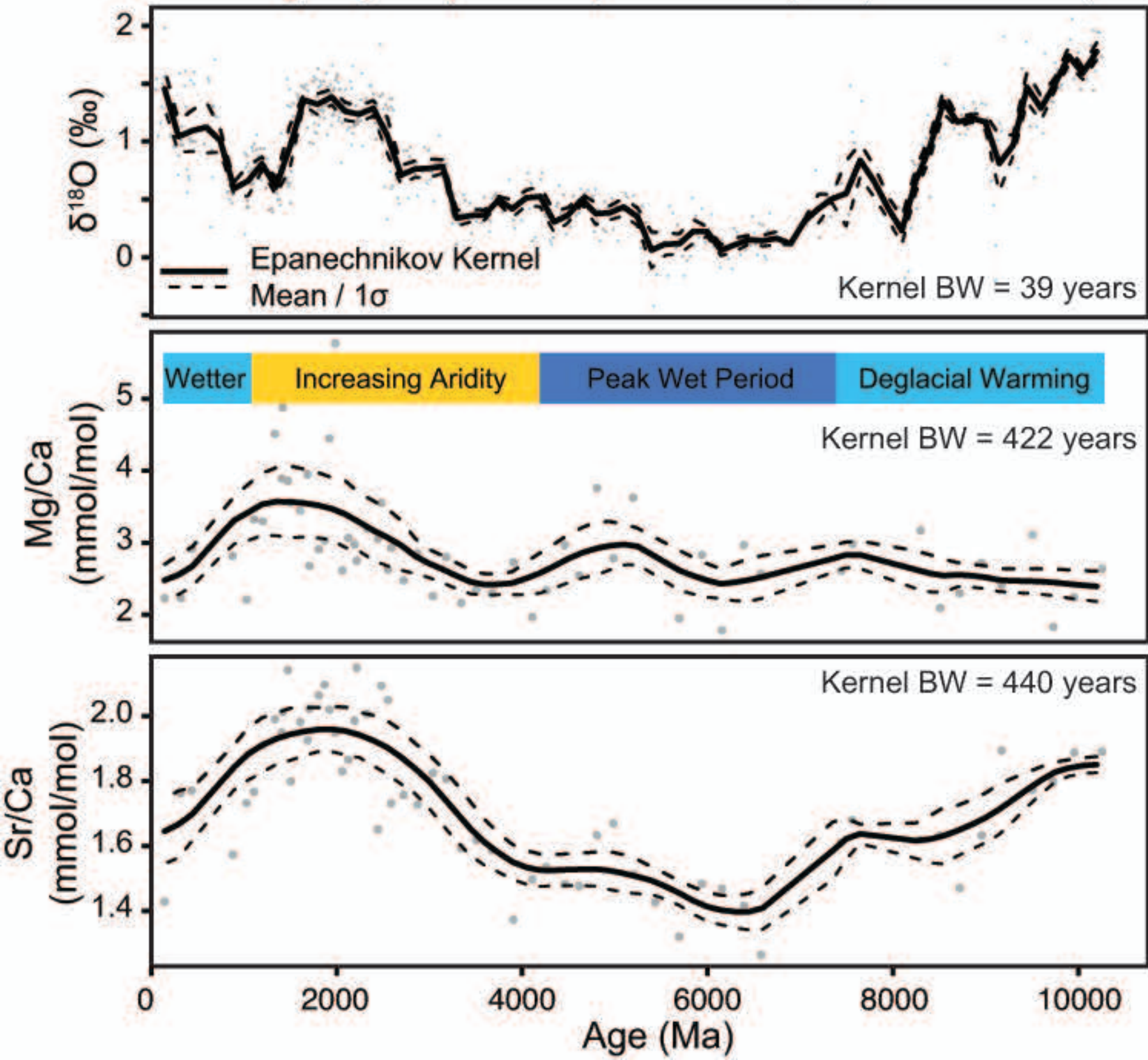
1139 Figure A2. Annual weighted precipitation $\delta^{18}\text{O}$ and mean annual temperature from the Global
1140 Network in Precipitation Data (GNIP) as compiled by the Stable Water Isotope Intercomparison
1141 Group (SWING). Following Rozanski and other (1993) we calculate slope of the temperature vs.
1142 weighted precipitation $\delta^{18}\text{O}$ for the mid and high latitude ($> 23^\circ$) sites (grey), and tropics (black).
1143 We only use the empirical regression (slope and uncertainty) for the tropics in modeling of Lake
1144 Miragoane temperature changes. For the Songliao Basin we use the original regression of
1145 Rozanski and others (1993) of $0.58 \text{‰}/^\circ\text{C}$.

1146

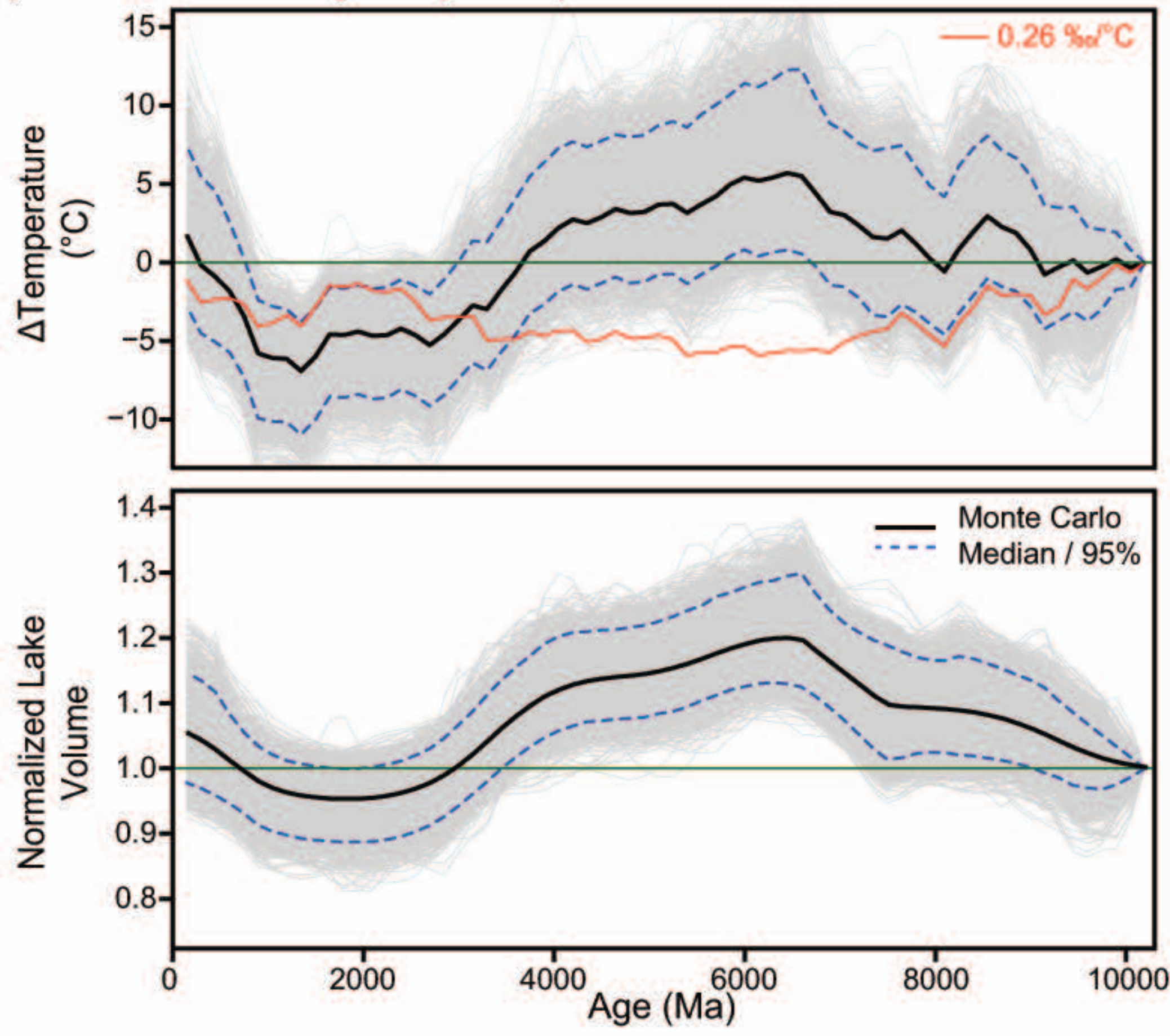


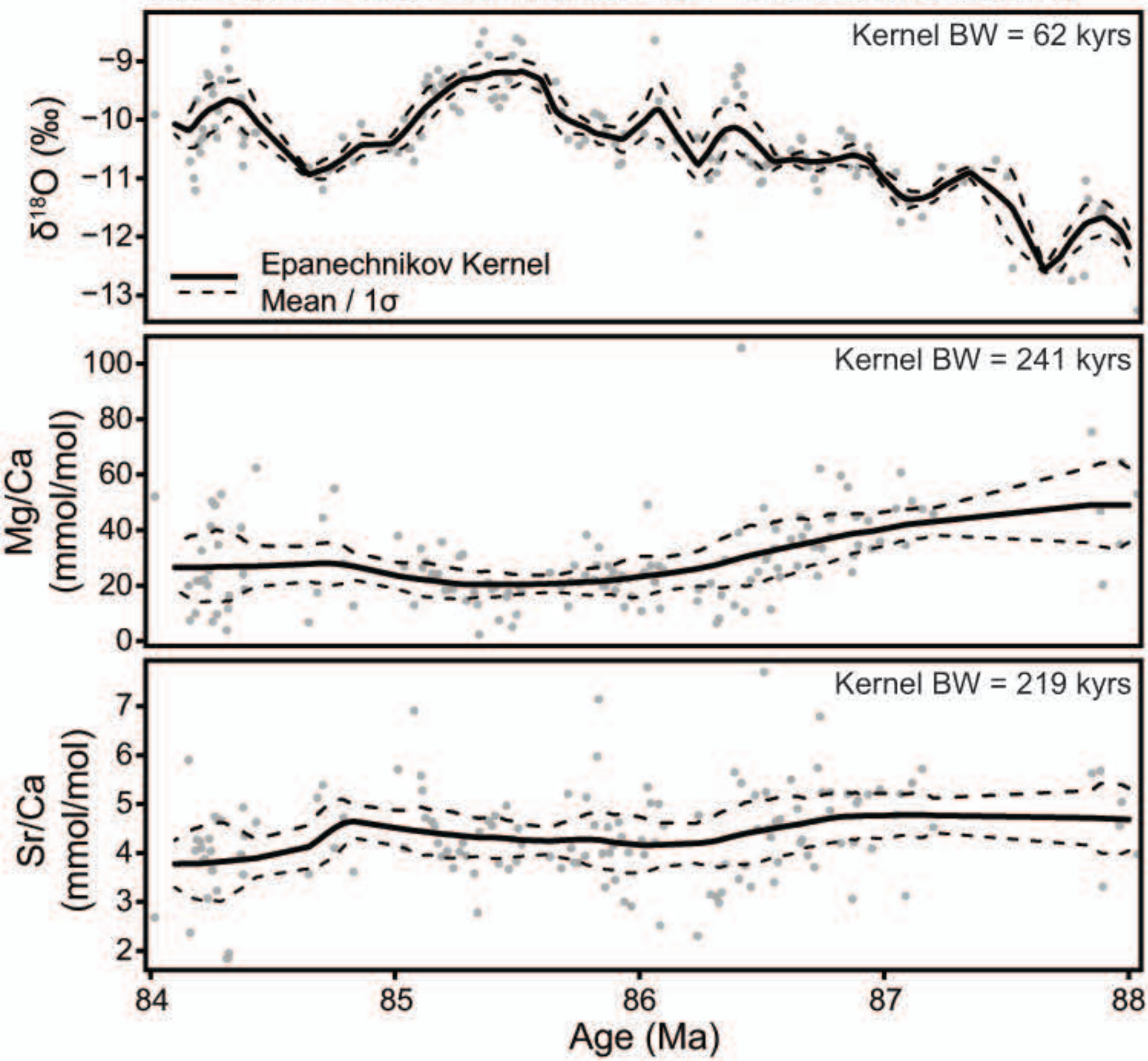
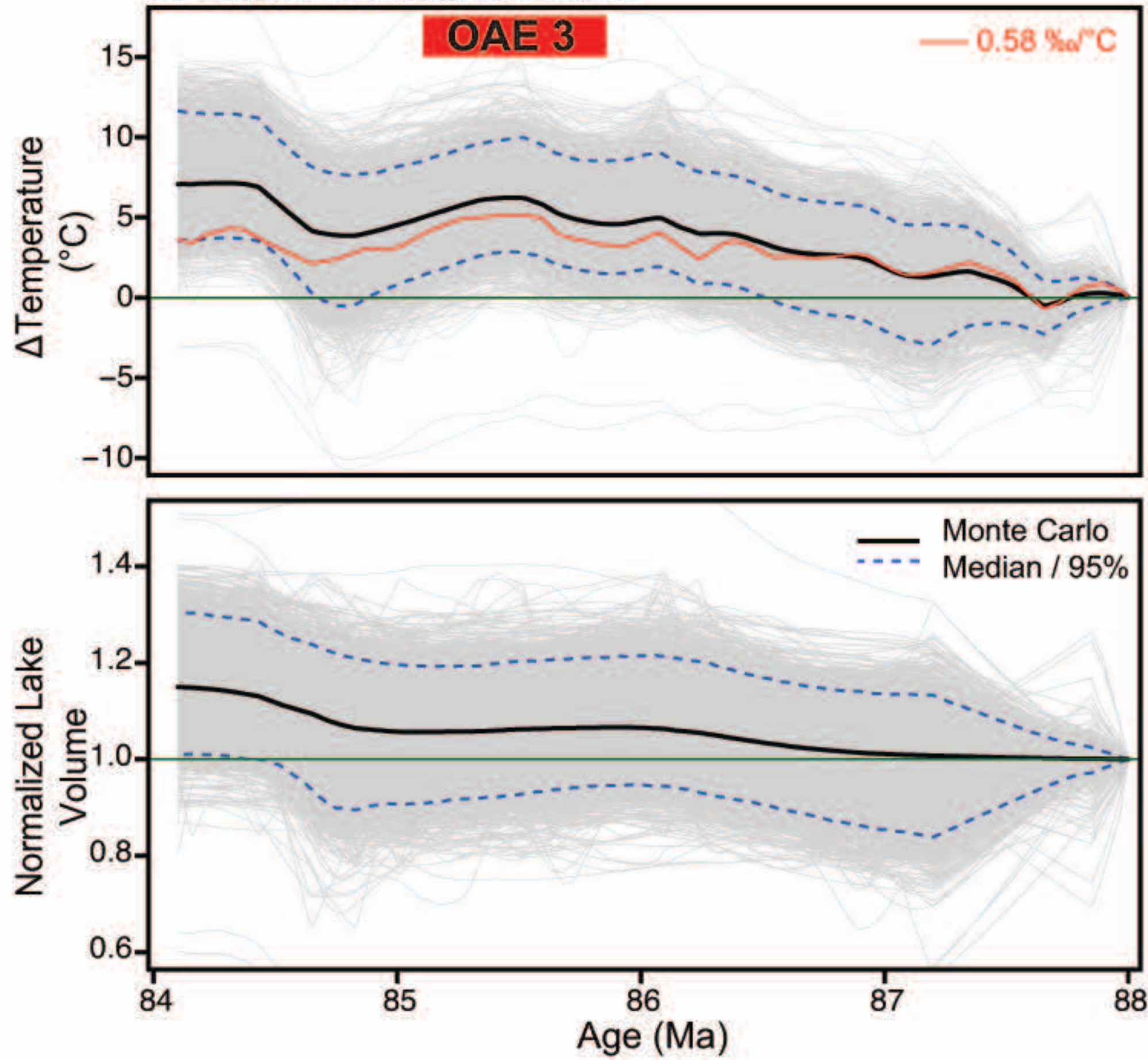


A. Lake Miragoane, Haiti (*Candona* sp. - Hodell et al., 1991; Curtis and Hodell, 1993)

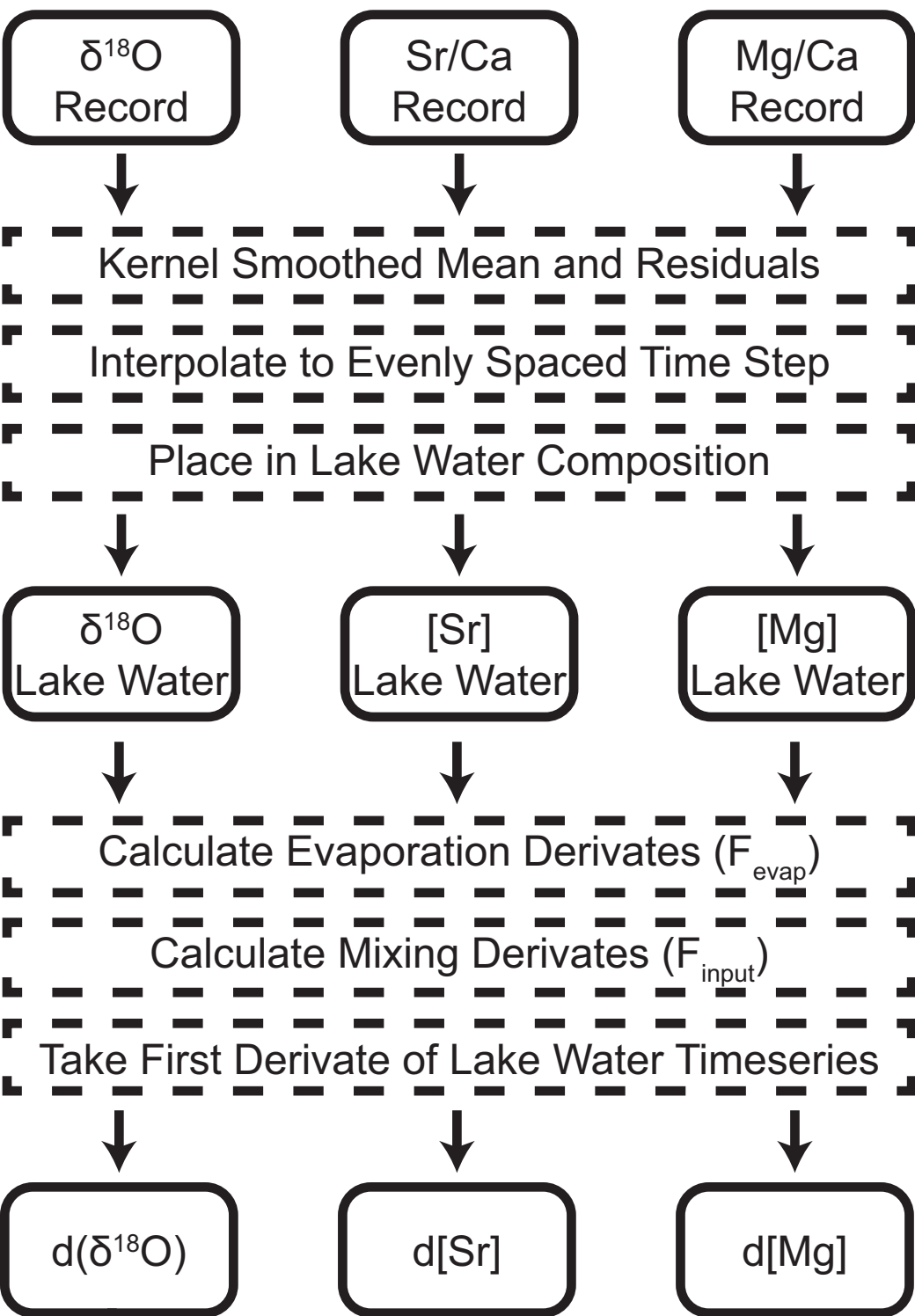


B. Lake Miragoane HyBIM Output

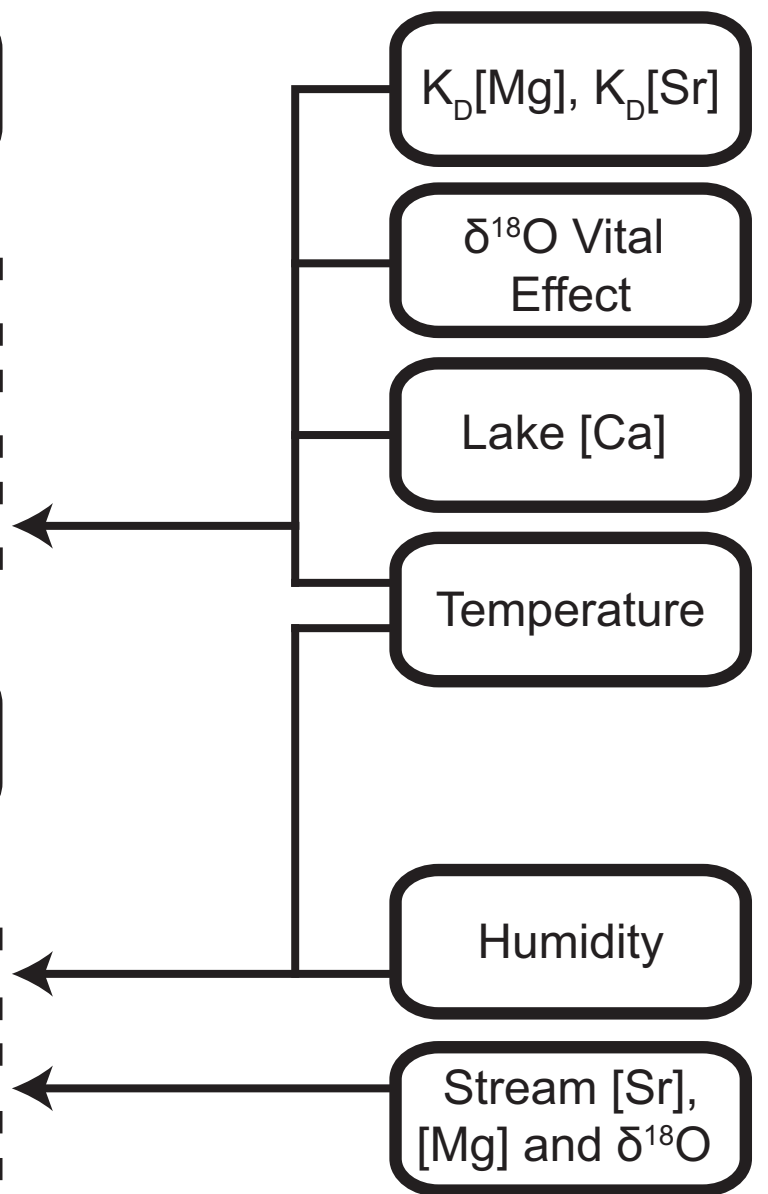


A. Songliao Basin, China (*Cypridea* sp. - Chamberlain et al., 2013)**B. Songliao Basin HyBIM Output**

Input Dataset



Input Parameters



$$\begin{bmatrix} \frac{\partial(\delta^{18}\text{O})}{\partial T} & \frac{\partial(\delta^{18}\text{O})}{\partial F_{\text{evap}}} & \frac{\partial(\delta^{18}\text{O})}{\partial F_{\text{input}}} \\ \frac{\partial[\text{Sr}]}{\partial T} & \frac{\partial[\text{Sr}]}{\partial F_{\text{evap}}} & \frac{\partial[\text{Sr}]}{\partial F_{\text{input}}} \\ \frac{\partial[\text{Mg}]}{\partial T} & \frac{\partial[\text{Mg}]}{\partial F_{\text{evap}}} & \frac{\partial[\text{Mg}]}{\partial F_{\text{input}}} \end{bmatrix}^{-1} \times \begin{bmatrix} d(\delta^{18}\text{O}) \\ d[\text{Sr}] \\ d[\text{Mg}] \end{bmatrix} = \begin{bmatrix} dT \\ dF_{\text{evap}} \\ dF_{\text{input}} \end{bmatrix}$$

Partial Derivatives Solution

Solve for dT , dF_{evap} and dF_{input} for each time step

