An improved approach to age-modeling in deep time: Implications for the Santa Cruz Formation, Argentina

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ABSTRACT

Accurate age-depth models for proxy records are crucial for inferring changes to the environment through space and time, yet traditional methods of constructing these models assume unrealistically small age uncertainties and do not account for many geologic complexities. Here we modify an existing Bayesian age-depth model to foster its application for deep time U-Pb and 40Ar/39Ar geochronology. More flexible input likelihood functions and use of an adaptive proposal algorithm in the Markov Chain Monte Carlo engine better account for the age variability often observed in magmatic crystal populations, whose dispersion can reflect inheritance, crystal residence times and daughter isotope loss. We illustrate this approach by calculating an age-depth model with a contiguous and realistic uncertainty envelope for the Miocene Santa Cruz Formation (early Miocene; Burdigalian), Argentina. The model is calibrated using new, high-precision isotope dilution U-Pb zircon ages for stratigraphically located interbedded tuffs, whose weighted mean ages range from ca. 16.78 ± 0.03 Ma to 17.62 ± 0.03 Ma. We document how the Bayesian age-depth model objectively reallocates probability across the posterior ages of dated horizons, and thus produces better estimates of relative ages among strata and variations in sedimentation rate. We also present a simple method to propagate age-depth model uncertainties onto stratigraphic proxy data using a Monte Carlo technique. This approach allows us to estimate robust uncertainties on isotope composition through time, important for comparisons of terrestrial systems to other proxy records.

INTRODUCTION

Placing measurements of proxy records (e.g., fossils, geochronometric data, pollen or phytolith abundances) in a broader geochronologic context is crucial for inferring environmental and faunal variations in space and time. For proxy records where stratigraphic position is known, chronology construction relies on both accurate and precise age determinations and an age-depth model that describes the relationship between stratigraphic position and time. This process is complicated by the underlying uncertainties in both the age determinations and the complex nature of sediment accumulation. Furthermore, datable materials are often intermittently distributed and are not necessarily co-located with the proxy record of interest, resulting in uncertainty in correlation and interpolation.

Considerable effort has been expended on how best to interpolate time from dated to undated stratigraphic positions, and a variety of proposed statistical methods have been proposed for this purpose (see reviews of: Blaauw and Heegaard, 2012; Parnell et al., 2011). Broadly, these methods can be split into two categories: classical and Bayesian models. Classical age-depth modeling encompasses a variety of deterministic linear, spline, and polynomial interpolation methods that aim to fit a smooth curve that relates stratigraphic position to age. The resulting models do not necessarily pass through each measured age, instead they are fit as closely as possible to each point, usually by a least squares approach (Blaauw and Heegaard, 2012). With the addition of Monte Carlo methods to simulate the underlying uncertainties in age, probabilistic classical models may produce satisfactory chronologies. However, they have several limitations. First, classical models do not explicitly consider stratigraphic relationships among samples and may produce chronologies that violate superposition and imply negative accumulation rates (See fig. 6 in Blaauw and Heegaard, 2012). Second, these methods often underestimate the uncertainties associated with undated positions (Blaauw et al., 2018; De Vleeschouwer and Parnell, 2014).

Bayesian inference offers an alternative to the classical approach by combining data (age determinations) and prior information (stratigraphic positions) to generate a satisfactory probabilistic posterior chronology. Originally developed for radiocarbon calibration and chronology construction (Blaauw and Christen, 2005; Bronk Ramsey, 2008; Haslett and Parnell, 2008), Bayesian age-depth modeling has become increasingly applied to other types of geochronologic data (De Vleeschouwer and Parnell, 2014; Sahy et al., 2015; Wotzlaw et al., 2018).

In this paper we introduce a modified version of an existing Bayesian age-depth model, Bchron (Haslett and Parnell, 2008), for use with U-Pb, 40Ar/39Ar, and other deep time geochronologic data. We then illustrate our approach for the Miocene (Burdigalian) Santa Cruz Formation of southern Argentina (Fig. 1). We use our new dates, cast within a Bayesian framework, as a test case to address two broad questions. First, how
does the inclusion of prior information affect the interpretation of the non-symmetric uncertainties that arise from the analysis of several individual mineral grains (e.g., zircon, sanidine)? Second, how can the significant uncertainties associated with age-depth models be considered in the interpretations of proxy records?

**BAYESIAN MODELING**

Bayesian models attempt to estimate the probable values of unknown parameters based on prior information about these parameters, which can be conditioned by observed data, or likelihoods. The relationship between these terms is formalized in Bayes' theorem:

\[ P(\theta | x) \propto P(x | \theta) \times P(\theta). \]  

(1)

The first term on the right-hand side of Equation 1 is the conditional probability of the data given the proposed parameters, i.e., how probable are our data (x; age determinations) given a proposed parameter (θ; model age). The second term is the probability associated with any prior knowledge of the parameters (θ), i.e., for our example, how constraints such as stratigraphic superposition and/or assumptions of sedimentation rate and its variability affect the probability of the proposed age parameters (θ). The left-hand term is the posterior conditional probability of the proposed parameters, i.e., what is the most probable age (θ) given our data (i.e., the radiometric age determinations) and our prior knowledge (stratigraphic position, sedimentation rate variability) interact.

In most cases Bayes’ theorem cannot be solved analytically, so we instead generate a representative sample of the posterior distribution using Markov Chain Monte Carlo (MCMC) methods. MCMC uses a variety of probabilistic proposal algorithms to produce a random sample of the posterior distribution. Given a large enough sample size and adequate exploration of parameter space, this sample should be representative of the “true” posterior distribution and should have the same underlying summary statistics (Kruschke, 2015).

**Bayesian Age-Depth Modeling with Bchron**

Originally designed for radiocarbon calibration and age-depth modeling, Bchron is available as an open source R package (Haslett and Parnell, 2008). Bchron generates an age model, given specific age determinations, associated uncertainties, and stratigraphic positions. The model treats sedimentation as a series of accumulation events of varying duration and amount, where the number of accumulation events is drawn from a Poisson distribution and the amount of accumulation is drawn from a gamma distribution. These two processes are related using a compound Poisson-gamma distribution to describe the prior probability of the sedimentation events (Haslett and Parnell, 2008). In addition to the parameters associated with age determinations, Bchron uses two hyperparameters (μ, ψ) to control the mean and dispersion of the compound Poisson-gamma distribution. Because these hyperparameters (μ, ψ) are calculated over the entire section, accumulation paths that have roughly the same mean accumulation rate are effectively favored. This method results in a model that is piecewise linear and allows for a wide variety of possible accumulation paths (Fig. 2).

A piecewise linear process is desirable for several reasons. First, the process is monotonically increasing such that stratigraphically higher positions are always younger than those below, thus capturing the fundamental stratigraphic principle of superposition. Second, the process allows for a wide range of sedimentation paths and there is no a priori assumption of smoothly varying sedimentation rates. While classical methods often assume that accumulation rates vary only at dated positions or vary smoothly in between, a piecewise linear process with a varying number of change points allows for segments that imply near-zero (disconformity-like) to very rapid accumulation rates (Haslett and Parnell, 2008). Confidence intervals of chronologies based on classical methods often exhibit a waist or hourglass effect where model uncertainties counterintuitively decrease as distance from dated positions increases, underestimating uncertainty at these positions (De Vleeschouwer and Parnell, 2014; Telford et al., 2004). Conversely, by allowing the number of sedimentation events to vary by both duration and amount, Bchron model probabilities are presented as a highest density interval (HDI), which is similar to a confidence interval but makes no prior assumptions about the distribution shape. These HDI’s take on a sausage-like shape where uncertainty increases with distance from dated positions. This phenomenon captures the expectation that uncertainty should increase in areas poorly constrained by data.

**GEOLOGIC SETTING OF SANTA CRUZ FORMATION SAMPLES**

We focus on the Santa Cruz Formation because it is one of the most fossiliferous sedimentary sequences in South America and provides an unparalleled opportunity to link paleoclimatic and faunal evolution immediately prior to the mid-Miocene climatic optimum (Vizcaíno et al., 2012b). The formation is part of the Miocene infill of the South American Austral Basin. It trends NW-SE, is bounded by the Patagonian...
Andes in the west and the Deseado Massif in the northeast and is open to the Atlantic Ocean toward the east and southeast. During the Miocene, Andean uplift and crustal loading drove an increase in accommodation space, allowing the accumulation of the terrestrial deposits of the Santa Cruz Formation (Blisniuk et al., 2005; Bown and Fleagle, 1993; Cuitiño et al., 2019; Fosdick et al., 2013; Marshall, 1976). Outcrops of these Santa Cruz Formation deposits are extensive, with exposures from the Andean foothills to the Atlantic coast (Blisniuk et al., 2005; Cuitiño and Scasso, 2010; Fleagle et al., 2012; Malumian et al., 1999; Marshall, 1976; Tauber, 1994, 1997). While geographically widespread, the exposures are discontinuous, and depositional idiosyncrasies make some sections less amenable to dating. However, because such large areas of the Santa Cruz Formation are exposed, age controls from multiple localities can be integrated using lithological and tephrochronological correlations (see fig. 2.2 in Perkins et al., 2012).

There has been considerable effort to constrain the age of the Santa Cruz Formation and its fossil localities. K-Ar dates placed the Santa Cruz Formation in the late-early to middle Miocene (Everden et al., 1964; Marshall et al., 1977) and at 16–17 Ma (Marshall et al., 1986). $^{40}$Ar/$^{39}$Ar analyses for coastal exposures included a range from ca. 19.3 to ca. 16.2 Ma (Fleagle et al., 1995) and an age of 16.68 ± 0.11 Ma for a tuff from the Killik Aike Norte locality (Tejedor et al., 2006). Dates from western exposures ranged from 22.4 to 14.2 Ma (Blisniuk et al., 2005). To synthesize these ages, Perkins et al. (2012) and Fleagle et al. (2012) reported new $^{40}$Ar/$^{39}$Ar ages for several tuffs, recalibrated previous dates, correlated tuffs (and their ages) across many Santa Cruz Formation localities using tephrochronology and constructed a chronostratigraphic framework for much of the Santa Cruz Formation. More recently Cuitiño et al. (2016) reported four U-Pb ages from strata exposed along the Río Bote and Río Santa Cruz, allowing correlation from western to eastern exposures.

**MATERIALS AND METHODS**

**U-Pb Geochronology**

We analyzed tuffs from six Santa Cruz Formation localities: Cañadón de las Vacas, Rincón del Buque 3, Cerro Observatorio, Killik Aike Norte, Cabo Buen Tiempo, and Puesto Estancia La Costa (Fig. 1; Table 1). Combined with the stratigraphic framework of Perkins et al. (2012), our new mapping and stratigraphic sections allow correlations among these sites (Fig. 3). We follow the abbreviations of Perkins et al. (2012) for locality and tuff names whenever possible to facilitate comparisons of our ages with theirs.

All mineral separations and isotope analyses took place in the Boise State Isotope Geology Laboratory, Boise, Idaho, USA. Zircon crystals were separated from each sample using density and magnetic methods. The resulting crystal concentrates were heated in a muffle furnace at 900 °C for 60 h to anneal minor radiation damage and prepare crystals for chemical abrasion. After annealing, individual grains were hand-picked, mounted in epoxy, polished to their centers using silicon carbide lapping film and 0.3 μm alumina, and imaged by cathodoluminescence (CL).

**TABLE 1. GPS COORDINATES AND ELEVATION, COMPOSITE STRATIGRAPHIC POSITION, AND WEIGHTED MEAN AGES FOR ALL SAMPLES FROM THE SANTA CRUZ FORMATION, ARGENTINA**

<table>
<thead>
<tr>
<th>Sample</th>
<th>Locality</th>
<th>Latitude</th>
<th>Longitude</th>
<th>GPS elevation</th>
<th>Stratigraphic position</th>
<th>Weighted mean age</th>
</tr>
</thead>
<tbody>
<tr>
<td>CV-10</td>
<td>CV</td>
<td>–50.55754</td>
<td>–69.15467</td>
<td>195</td>
<td>179</td>
<td>16.825 ± 0.036</td>
</tr>
<tr>
<td>Toba Blanca</td>
<td>CV</td>
<td>–50.5572</td>
<td>–69.15482</td>
<td>185</td>
<td>175</td>
<td>16.868 ± 0.032</td>
</tr>
<tr>
<td>KARG-15-01</td>
<td>CV</td>
<td>–50.5646</td>
<td>–69.15071</td>
<td>181</td>
<td>161</td>
<td>16.850 ± 0.022</td>
</tr>
<tr>
<td>KARG-15-09</td>
<td>CV</td>
<td>–50.6550</td>
<td>–69.21211</td>
<td>96</td>
<td>84.5 ± 2.5</td>
<td>17.006 ± 0.039</td>
</tr>
<tr>
<td>CV-13</td>
<td>CO</td>
<td>–50.6016</td>
<td>–69.08627</td>
<td>–</td>
<td>48.25 ± 3.13</td>
<td>17.615 ± 0.026</td>
</tr>
<tr>
<td>KAN1</td>
<td>KAN</td>
<td>–51.5747</td>
<td>–69.44655</td>
<td>4.9</td>
<td>–</td>
<td>16.996 ± 0.025</td>
</tr>
<tr>
<td>KARG-15-08</td>
<td>CBT</td>
<td>–51.5284</td>
<td>–68.95529</td>
<td>41</td>
<td>–</td>
<td>16.949 ± 0.030</td>
</tr>
<tr>
<td>KARG-15-12</td>
<td>PLC</td>
<td>–51.19278</td>
<td>–68.89952</td>
<td>105</td>
<td>–</td>
<td>16.783 ± 0.051</td>
</tr>
</tbody>
</table>

Notes: CV—Cañadón de las Vacas; CO—Cerro Observatorio; KAN—Killik Aike Norte; CBT—Cabo Buen Tiempo; PLC—Puesto Estancia La Costa; masl—meters above sea level.

After imaging, we analyzed 30–40 crystals from each sample via laser ablation–inductively coupled plasma–mass spectrometry (LA-ICP-MS) using a ThermoElectron X-Series II quadrupole ICP-MS and a New Wave Research UP-213 Nd:YAG UV (213 nm) laser ablation system. Details of the LA-ICP-MS methodology are reported in Macdonald et al. (2018). LA-ICP-MS $^{206}$Pb/$^{207}$U, $^{207}$Pb/$^{206}$Pb ages, U content, CL zonation pattern, and visual clarity were then used to select single zircon grains for chemical abrasion–isotope dilution–thermal ionization mass spectrometry (CA-ID-TIMS) analysis. Individual crystals were chemically abraded in concentrated hydrofluoric acid at 180 °C for 12 h to remove mineral

Figure 3. Correlation diagram for Santa Cruz Formation, Argentina, localities considered in this study. The geographic location of each locality is shown in Figure 1. Colored stratigraphic columns are used to form the composite section shown in Figure 5. Stratigraphic columns for Cabo Buen Tiempo (CBT), Killik Aike Norte (KAN), and Puesto Estancia La Costa modified from Perkins et al. (2012). CO—Cerro Observatorio; CV—Cañadón de las Vacas; CA—Corrigüe Aike.
inclusions and mitigate open system behavior (Mattinson, 2005). Residual crystals were then spiked with the ET535 isotope dilution tracer (Condon et al., 2015; McLean et al., 2015) and processed for chemical abrasion isotope dilution thermal ionization mass spectrometry (CA-IDTIMS; Macdonald et al., 2018). Isotope ratios were measured using an IsotopX Phoenix X62 or Isoprobe-T mass spectrometer; U-Pb dates and uncertainties were calculated using the methods of Schmitz and Schoene (2007) and the U decay constants of Jaffey et al. (1971). Errors for calculated weighted means are reported in the form ± X(Y)[Z] where X is the analytical uncertainty, Y is the combined analytical and tracer (EARTHTIME 535; Condon et al., 2015; McLean et al., 2015) uncertainties, and Z is the combined analytical, tracer, and decay constant uncertainties. Repeated measurements of the EARTHTIME ET100 U-Pb isotope ratio standard solution are reported in Table DR5*, and document no significant overdispersion relative to the propagated uncertainties of the analyses, while demonstrating agreement with the long-term average values measured in the Boise State University Isotope Geology Laboratory.

Model Modifications

In this study we modified the Bchron compound Poisson-gamma age-depth model for use with U-Pb and 40Ar/39Ar data in deep time stratigraphic contexts. Our model is implemented as an R package (R Core Team, 2019), available for download at https://github.com/robintrayler/modifiedBChron. Here we outline our modifications.

Assignment of Age Uncertainties

We allow individual dates to be grouped to form complex probability density functions, reproducing the practice in both U-Pb and 40Ar/39Ar geochronology of convolving many single crystal or spot analyses into a single age model. Modern high precision dates on single mineral crystals from volcanic rocks often demonstrate dispersion beyond analytical uncertainty (Jicha et al., 2016; Rivera et al., 2013). Consequently, the resulting age probability estimation for each dated horizon is a complex function that can be modeled as a summed probability density plot or kernel density estimate (Vermeech, 2012), which we will generically call a “probability distribution.” We have included the ability to combine individual dates based on a grouping variable (e.g., from the same stratigraphic horizon). Within each group, individual dates and uncertainties are specified by the user as either normal (or uniform) distributions, and then summed within the algorithm on the basis of the grouping variable to form the final probability distributions for each dated horizon. By grouping data in this way, the user can model arbitrarily complex radioactive age, magnetic reversal, or even detrital zircon maximum depositional age likelihood distributions.

Markov Chain Monte Carlo Implementation

We implement an adaptive Markov Chain Monte Carlo algorithm to remove the need for data rescaling. Bchron and our model use a Metropolis-Hastings algorithm to evaluate Bayes’ equation and produce a posterior sample for each model parameter. Briefly, for each iteration of each Markov chain a new parameter is proposed from a Gaussian proposal distribution centered on the current parameter value. The proposed parameter and current parameter are compared and accepted or rejected probabilistically (Brooks et al., 2011; Chib and Greenberg, 1995; Kruschke, 2015). In effect the algorithm randomly walks through the parameter space. The efficiency of this algorithm depends heavily on an appropriately scaled proposal distribution. However, without a priori information about the target distribution, selecting an appropriately scaled proposal distribution is difficult. Bchron addresses this problem by rescaling the input data (age determinations, age uncertainties, stratigraphic positions) to limit the possible size of the proposal distribution. While the restricted time and spatial scales of radiocarbon chronologies are amenable to this approach, it is inflexible for deeper time data that may be presented in thousands (ka), millions (Ma), or billions (Ga) of years as they require vastly different scaling factors. A variety of adaptive proposal algorithms have been developed to address this problem (e.g., Christen and Fox, 2010; Gelman et al., 1996; Haario et al., 2001; Roberts and Rosenthal, 2009). Here we use the adaptive proposal algorithm of Haario et al. (1999) to ensure that the parameter space (i.e., the set of all possible values for a parameter) is efficiently explored. In this method the proposal distribution for each dated horizon is defined as:

\[ \theta_i = N(\theta_i, c^2 \sigma^2_i), \]  

where \( \theta_i \) is the current model age in the Markov Chain for a specific horizon, \( \theta_i \) is the proposed model age at the same horizon, \( \sigma^2_i \) is the variance of the previous \( h \) iterations in the Markov Chain, and \( c^2 \) is an empirically determined constant scaling factor. We use \( c^2 = 2.4 \) as recommended by Gelman et al. (1996) and Haario et al. (1999). In effect, the variance of each model parameter is monitored during each simulation and a unique proposal distribution for each parameter is adjusted accordingly.

Outlier Rejection

We have removed automated outlier rejection. Instead we prescreen our data for outliers using a variety of established criteria based on the physical mechanisms of crystal growth and open system behavior in volcanic rocks. Biased dates for mineral crystals primarily arise from three processes. First, open system behavior resulting from the loss of radiogenic daughter isotopes biases analyses to apparently younger ages. Second, mineral inclusions within a crystal may have anomalous daughter to parent isotope ratios and/or initial daughter contents, which contaminate and bias the resulting dates to apparently older ages. Finally, inheritance or recycling of geologically older crystals produces dates that are older than the erasable age of the target magmatic event. A variety of analytical methods have been developed to minimize these systematic outliers for U-Pb and 40Ar/39Ar data. For zircon crystals, chemical abrasion prior to analysis reduces the influence of open system behavior and contamination by selectively removing inclusions and damaged portions of the zircon lattice most susceptible to loss of radiogenic lead (Mattinson, 2005). When lead loss is intransigent, even after chemical abrasion, its effect may be identified and those samples manually excluded, through comparisons of co-variance of 206Pb/238U and 204Pb/206Pb (Wetherill, 1956, 1963). Likewise, the development of the step heating method for 40Ar/39Ar, coupled with careful examination of the resulting age spectrum for argon-bearing minerals using a plot of cumulative 39Ar versus age and the inverse isochron diagram allow open system behavior in these systems to be monitored (McDougall and Harrison, 1999).

For both dating systems, crystal recycling or inheritance, either from much older country rock (xenocrysts) or slightly older volcanic materials from the same volcanic system (antecrysts) may produce dates older than the actual time of eruption. Xenocrysts that are significantly older than the dominant age mode are trivial to reject. In some cases, slightly older antecrysts may be removed by the application of several statistical rejection criteria (Michel et al., 2016), although these effects are often subtle. We focus here on the ability of Bayesian age modeling to objectively mitigate these antecryst effects by quantitatively rejecting older age modes using superpositional constraints.

*GSA Data Repository item 2019241, Figures DR1–DR4; Appendix 1, example code; and Tables DR1–DR5, is available at http://www.geosociety.org/datarepository/2019 or by request to editing@geosociety.org.

Geological Society of America Bulletin
RESULTS

U-Pb CA-ID-TIMS

Summary location and age information for each sample are listed in Table 1, while the full data acquired by LA-ICP-MS (Tables DR3 and DR4) and CA-ID-TIMS (Table DR5) are reported in the supplemental material.

Killik Aike Norte (KAN)

Killik Aike Norte (KAN: 51° 34′ S, 69° 25′ W) is a series of exposures along the north banks of the Río Gallegos estuary, located ~100 km south of Cerro Observatorio along the Atlantic coast. The Santa Cruz Formation is exposed in the walls of a deep canyon that enters the river channel from the north, with continuous exposures along the northern banks of the river itself (Marshall, 1976). Tejedor et al. (2006) illustrated a stratigraphic column and reported an ⁴⁰Ar/³⁹Ar age of 16.68 ± 0.05 Ma (recalibrated by Perkins et al., 2012) for a vitric tuff from KAN. However, analysis of a pumice clast within the tephra gives an ⁴⁰Ar/³⁹Ar age of 17.06 ± 0.07 Ma (Perkins et al., 2012). We collected a new sample of the KAN tuff for analysis to address this discrepancy.

KAN-1

CL imaging of zircon from the KAN-1 tuff revealed predominantly equant, oscillatory zoned crystals. A minority of grains exhibited an elongate, prismatic morphology but were otherwise similar to the equant population. CL-dark inherited cores were common and avoided. Of 39 grains analyzed by LA-ICP-MS, 24 grains (61%) returned Miocene ²⁰⁶Pb/²³⁸U ages (Table DR4). Of these grains, fourteen grains were selected for CA-ID-TIMS analysis on the basis of CL zoning patterns and LA-ICP-MS ²⁰⁶Pb/²³⁸U date. Of these, four analyses had a radiogenic to common lead ratio <1 and were discarded. Of the remaining crystals, six analyses were concordant, of equivalent age, and returned a weighted mean ²⁰⁶Pb/²³⁸U date of 16.996 ± 0.014(0.017)[0.025] Ma (MSWD = 0.43; n = 5), which is interpreted as estimating the eruption age of the tuff.

CV-10

CL imaging of zircon from the CV-10 tuff revealed a uniform population of prismatic, oscillatory zoned crystals. A minority of grains contained CL distinct rounded cores that were avoided in all subsequent analyses. Of 38 grains analyzed by LA-ICP-MS, 37 grains (97%) returned Miocene ²⁰⁶Pb/²³⁸U ages (Table DR4). Five grains were selected for CA-ID-TIMS analysis on the basis of LA-ICP-MS ²⁰⁶Pb/²³⁸U date and CL zoning. These analyses were concordant, of indistinguishable isotope ratios, and returned a weighted mean ²⁰⁶Pb/²³⁸U date of 16.850 ± 0.009(0.013)[0.022] Ma (MSWD = 0.43; n = 5), which is interpreted as estimating the eruption age of the tuff.

CV-13

CL imaging of zircon from the CV-13 tuff revealed a uniform population of elongate, prismatic, oscillatory zoned crystals. CL dark inherited cores were common and avoided. Of 30 grains analyzed by LA-ICP-MS, 21 grains (70%) returned Miocene ²⁰⁶Pb/²³⁸U ages (Table DR4). Sixteen grains were selected for CA-ID-TIMS analysis. Two analyses had a radiogenic to common lead ratio <1 and were discarded. Four additional grains with ²⁰⁶Pb/²³⁸U dates >19 Ma were also set aside as inherited detritus. Five of the nine remaining grains yielded concordant and indistinguishable isotope ratios with a weighted mean ²⁰⁶Pb/²³⁸U date of 17.620 ± 0.015(0.017)[0.026] Ma (MSWD = 1.44; n = 5), which is interpreted as the eruption age of the tuff. Four slightly older grains were excluded from the weighted mean calculation and are assumed to represent either detrital or pre-eruptive grains.

Cabo Buen Tiempo (CBT)

At Cabo Buen Tiempo (51° 34′ S, 68° 57′ W), Santa Cruz Formation strata (including fossiliferous levels and numerous tuffs) are exposed on a tidal platform at low tide and in an adjacent sea cliff. Perkins et al. (2012) correlated several CBT tuffs to other localities. The only direct date of a CBT tuff is imprecise (<17.73 Ma; Perkins et al., 2012). We collected a sample of the lowest exposed tuff (~41 m above sea level) at Cabo Buen Tiempo (KARG-15-08). Based on the stratigraphic scheme of Perkins et al. (2012), this is likely the KAN-2 tuff.

KAN-2

CL imaging of zircon from the KARG-15-08 tuff revealed a mixed population of elongate and equant, prismatic, oscillatory zoned crystals. Inherited cores were uncommon and avoided. Of 37 grains analyzed by LA-ICP-MS, 31 grains (84%) returned Miocene ²⁰⁶Pb/²³⁸U ages (Table DR4). Nineteen grains were selected for CA-ID-TIMS analysis. Six analyses had a radiogenic to common...
Figure 4. U-Pb Concordia and ranked age plots for all analyzed samples, Santa Cruz Formation, Argentina. Shaded symbols indicate analyses included in weighted mean calculations. The light gray band on ranked age plots indicates the weighted mean. All uncertainties are shown as $2\sigma$. CV—Cañadón de las Vacas; KAN—Killik Aike Norte.
mon lead ratio <1 and were rejected. An additional grain with a 206Pb/238U date of >19 Ma was also rejected as probable inheritance. Of the remaining twelve grains the six youngest grains are concordant and of indistinguishable isotope ratio, with a weighted mean 206Pb/238U date of 16.949 ± 0.022(0.023)[0.030] Ma (MSWD = 0.68; n = 6), which is interpreted as estimating the eruption age. Four slightly older grains were excluded from the weighted mean calculation and are assumed to represent either inheritance or an earlier period of zircon growth. Two other grains with very high 206Pb/238U date uncertainties (2σ > 0.15 Ma) were also excluded.

Rincón Del Buque (RB)

Located ~10 km S-SE of Cerro Observatorio and Cañadón de las Vacas, Rincón del Buque (50° 39’ S, 69° 12’ W) is a large half-moon shaped amphitheater (Marshall, 1976; Raigemborn et al., 2015; Vizcaíno et al., 2012a) exposing the Santa Cruz Formation as a series of benches and cliffs. We collected a single tuff (KARG-15-09) for analysis from Rincón del Buque 3 (RB3). This locality outcrops along the north of the Rincón Del Buque amphitheater at the border between Estancias Cañadón de las Vacas and Ototel Aike, Argentina.

KARG-15-09

CL imaging of zircon from the KARG-15-09 tuff revealed a mixture of equant and elongate, prismatic, oscillatory zoned crystals. Inherited cores and large inclusions are uncommon and avoided. Of 34 grains analyzed by LA-ICP-MS, 17 grains (50%) returned Miocene 206Pb/238U ages (Table DR4). Seventeen grains were selected for CA-ID-TIMS analysis. Eleven analyses had a radiogenic to common lead ratio of <1 and were avoided. Of 33 grains analyzed by LA-ICP-MS, 24 grains (72%) returned Miocene 206Pb/238U ages (Table DR4). Eight grains were selected for CA-ID-TIMS analysis. One grain had a radiogenic to common lead ratio of <1 and was discarded. Another grain with a 206Pb/238U date >18 Ma was set aside as inherited or detrital. The remaining seven grains are concordant and have indistinguishable isotope ratios, with a weighted 206Pb/238U date of 16.783 ± 0.047(0.048) [0.051] Ma (MSWD = 0.72; n = 6).

Model Validation

The goal of MCMC algorithms is to produce a posterior sample that is stable, representative, and reproducible (Kruschke, 2015). The underlying compound Poisson-gamma process of Bchron has been repeatedly validated. Using synthetic data, Haslett and Parnell (2008) showed that ~80–95% of model highest density intervals (HDIs) encompass the “true” accumulation path. Parnell et al. (2011) compared several Bayesian age-depth models, including Bchron, using three metrics; modal distance, proportion of contained probability distributions, and the Kulback-Leiber divergence measure. Briefly, modal distance is the difference between the mode of a model posterior distribution and the mode of the input likelihoods. Kulback-Leiber divergence is similar to modal distance except that it compares the entire probability distribution instead of summary statistics (i.e., modes). Both modal distance and Kulback-Leiber divergence calculations suggest that Bchron does not diverge unnecessarily from the points where age is best understood. The proportions of contained probability distributions are calculated using a leave-one-out cross validation, where individual age determinations are excluded from a data set. The resulting model is then compared to the excluded age. Parnell et al. (2011) showed that ~50% of excluded ages were completely contained within model 95% HDIs.

Our modified model uses the same underlying statistical framework as Bchron and repeated comparisons revealed only small differences between Bchron and our modified version, which are comparable to those observed among individual Bchron runs (Fig. DR1; see footnote 1). We therefore focused on examining the performance of our model across repeated model runs to ensure that our modifications do not affect model stability.

To assess model performance, we generated 500 individual simulations for the Santa Cruz Formation data set. Each simulation comprised 10,000 iterations with the initial 5000 steps discarded to allow the model to stabilize (i.e., burn-in). First, we examined the trajectory of each model parameter using trace plots (Fig. DR2; see footnote 1). Individual trace plots for each parameter stabilized quickly and mixed well. Comparing all 500 model simulations showed no visual difference between model runs for each parameter. Similarly, probability density estimates (kernel density estimates) of each model parameter were visually indistinguishable between simulations (Fig. DR3; see footnote 1). We also monitored variability in the lower bounds, upper bounds, and median of the 95% HDI across all model runs. The median was stable and varied only slightly (~±0.004 Ma; 2σ). The lower and upper bounds of the HDI also show little change among iterations (~±0.006 Ma; 2σ).

Modeling the Santa Cruz Formation

We developed two age-depth models for the Santa Cruz Formation, based on a composite stratigraphy of the CV locality, one using weighted mean ages, and another using the summed probability distributions of all analytically acceptable dates as inputs. For each model we included dates from CV (KARG-15-01, CV-10, Toba Blanca), and those from the nearby RB3 (KARG-15-09) and CO (CV-13) localities. The stratigraphic positions of these tuffs were projected into the CV composite by proportionally scaling the distance between marker beds of known stratigraphic position at each locality (Fig. 3). We also include 40Ar/39Ar ages for two tuffs at Cañadón de las Vacas (CO, CO3) previously reported by Perkins et al. (2012).

When weighted mean ages were used as the data likelihood for each tuff (Fig. 5A), the median for each posterior age likelihood distribution differed from the input weighted mean ages by only a few thousand years (Table 2). In the upper section, where there is considerable overlap between weighted mean ages, median model ages were consistently younger (Fig. 6), as a consequence of the superposition model prior. Perhaps more importantly, posterior age uncertainties for each tuff were also reduced compared to weighted means by 10–20% (~0.01–0.04 Ma), reflecting the positive effects of each dated horizon on those nearby.
When we used the summed probability distribution as the likelihood input (Fig. 5B), the model results showed several differences compared to the weighted mean model. Median model ages were consistently shifted younger when compared to the median of the likelihood probability distribution. Once again, this effect was most common in the upper section where likelihood probability distributions overlap significantly. The magnitude of the shift is also greater with a maximum shift of 0.08 Ma for the median and 0.006 Ma and 0.04 Ma for the lower and upper bounds of the 95% HDI, respectively. The largest difference between the antecryst model and the final summed probability distribution model are in the lower part of the section and are likely attributable to the visibly older mode for sample CV-13. As this sample is stratigraphically lowest, superpositional constraints cannot reject these older dates. It should be noted, however, that these antecrysts are easily rejected using the methods discussed above. The inclusion of all antecrysts into a single model ultimately represents a worst-case scenario where there was no prescreening of data for outliers.

In both models, the model bounds (HDI's) were broadest in the area between the CV-13 and KARG-15-09 tuffs and were much larger than the HDI's of the tuffs. In the upper section where tuffs are more closely spaced, model HDI's were significantly smaller and similar to those of the tuffs themselves. Both the weighted mean model and summed probability distribution model showed the value of collecting high precision dates from closely spaced horizons.

We also investigated the sensitivity of the model to the inclusion of antecrysts (unshaded symbols in Fig. 4) that were otherwise excluded as outliers from our final data set. We generated an age-depth model using all dates for CV-13, CO, KARG-15-09, KARG-15-01, Toba Blanca, CV-10, and CO3. The antecryst model is broadly similar to the final summed probability distribution model (Fig. DR4; see footnote 1) with an average difference between the two of 0.02 Ma for the median and 0.006 Ma and 0.04 Ma for the lower and upper bounds of the 95% HDI, respectively. The largest difference between the antecryst model and the final summed probability distribution model are in the lower part of the section and are likely attributable to the visibly older mode for sample CV-13. As this sample is stratigraphically lowest, superpositional constraints cannot reject these older dates. It should be noted, however, that these antecrysts are easily rejected using the methods discussed above. The inclusion of all antecrysts into a single model ultimately represents a worst-case scenario where there was no prescreening of data for outliers.
Age modeling in deep time

Our results show the value of a hybrid approach, using traditional methods to screen grain dates for obvious outliers arising from diverse physical behaviors (inheritance, daughter isotope loss), while employing a Bayesian framework to condition the remaining dates into eruptive ages that are consistent with superpositional constraints and incorporate the variance seen in many magmatic mineral populations. The value of exploring the model’s effect on the input ages themselves is particularly evident in the upper portion of the composite section, where there is considerable overlap between the summed probability distributions of the closely spaced KARG-15-01, Toba Blanca, CV-10, and CO3 tuffs. In particular, the Toba Blanca (Fig. 6), CV-10, and CO3 tuffs have distinct younger modes that the Bechon algorithm favors over higher probability, older modes. In the lower section (KARG-15-09 and below), the less precise “Ar/Ar”/Ar dates for the CO tuff exhibits considerable overlap of its probability distribution with both the CV-13 (below) and KARG-15-09 (above) tuffs. Here again the influence of a superposition constraint is evident as the overlapping portions of the CO probability distribution are ignored by the model, reducing the HDI on the CO tuff by ~50%.

Alternatively, using weighted mean ages as a likelihood input produces an age model with lower overall uncertainties for interpolated points. It also results in slightly more rapid accumulation rates in the upper section, while accumulation rates in the lower section are nearly unchanged. Since the likelihood probability distributions are modeled as symmetrical Gaussian distributions, the three upper-most tuffs lack the younger high probability “tails” present in the summed probability distribution model. Consequently, the shift of posterior distributions for each of these tuffs toward younger ages is less pronounced than in the summed probability distribution model.

Accurately modeling an eruptive age in volcanic tuffs is complicated by physical processes of inheritance, crystal recycling, and prolonged periods of crystal growth in magma chambers, which often result in crystal populations with asymmetric probability distributions that may have distinctly younger or older tails (e.g., Toba Blanca, CV-10, CO3 tuffs). This dispersion is best captured using a summed probability model, but does lead to ambiguous cases where the dominant mode is older than the youngest grains. By allowing the consideration of stratigraphic relationships between samples, Bayesian age modeling identifies the younger, lower probability grains as the most probable eruptive age (Figs. 5C and 6). Conversely, some samples (KARG-15-01) are tightly grouped around an expectation value (mean) with no obvious structure to their probability distributions suggesting younger or older modes. In these cases, using weighted mean likelihoods results in overall improved model uncertainties. In principle, using weighted means as model inputs will likely result in higher “precision” results. However, weighted means of either whole crystal populations or a subset, are themselves a model of eruption age, which may or may not be appropriate given the structure of the data (Keller et al., 2018). In cases where the dispersion of crystal populations cannot be attributed solely to analytical uncertainty and in the absence of stratigraphic information, Bayesian methods still offer a useful alternative to determining eruptive age (Keller et al., 2018).

Age-depth modeling offers a complementary and alternative approach to interpreting dispersed crystal populations. Ultimately, the choice of either weighted means or summed probability distributions as likelihoods should be heavily influenced by the structure of the data.

**Using Age-Depth Models to Fine-Tune Ages**

While model results suggest that the ages of several tuffs require slight adjustments, overall our U-Pb ages and modeled posterior ages are consistent with previous radiometric ages for the Santa Cruz Formation. However, our data also include ages for five previously unanalyzed tuffs, which allows the refinement of correlations between localities.

The Toba Blanca is exposed in several coastal exposures of the Santa Cruz Formation (Tauben, 1994), and is distributed laterally over at least 500 km (Perkins et al., 2012), making it an important marker bed for the Santa Cruz Formation. Our weighted mean age for the Toba Blanca is within uncertainty of an “Ar/Ar” Ar age of 16.89 ± 0.05 Ma, previously published by Perkins et al. (2012). However, our age model results suggest that the Toba Blanca is slightly younger, with an age range of 16.80–16.84 Ma (Fig. 6) that is within uncertainty of both the weighted mean and the HDI of the summed probability distribution for the individual crystal ages. Likewise, model results indicate that both the CV-10 and CO3 tuffs are somewhat younger than their weighted mean ages. In all three cases their probability distributions have distinct younger tails, suggesting that the older modes do not represent the eruptive age and instead record a prolonged period of crystal growth or recycling from earlier magmatism. These complications present the question, what are the “correct” ages for these tuffs? In our view, given the observed dispersion in individual zircon ages, and the stratigraphic superposition relationship with a less complex tuff (i.e., KARG-15-01), the modeled posterior ages for the summed prob-
ability distributions (Table 2) are the most robust and realistic eruptive ages.

Implications for Correlations within the Santa Cruz Formation

Our data permit new correlations between the Cañadón de las Vacas composite section and other analyzed Santa Cruz Formation localities (Fig. 3). The weighted mean ages of the KAN-1 (Killick Aike Norte) and KARG-15-09 (Rincón del Buque 3) tuffs are statistically indistinguishable and we therefore propose these coeval tuffs represent a single eruptive event. Given that the Rincón del Buque 3 and Killick Aike Norte are separated by ~100 km, a new correlative tuff over this distance provides a valuable marker bed between the two localities. The sample KARG-15-08 (16.949 ± 0.030 Ma; CBT) was collected from the lowest exposed tuff at CBT and was previously identified as the KAN-2 tuff. The age of the tuff was inferred by Perkins et al. (2012) as ca. 16.9 Ma, which is supported by our results. Given that the KAN-2 tuff is also exposed ~5 m above the KAN-1 tuff at Killick Aike Norte (Perkins et al., 2012; Tejedor et al., 2006), our results add a new age constraint for this locality.

Using Age Models to Interpret Proxy Records

Exposures of the Santa Cruz Formation at Lago Posadas (~47° 60′ S, 71° 51′ W) preserve at least 500 m of stratigraphic section. Blisniuk et al. (2005) proposed an age range of ca. 22–14 Ma, but reevaluation of the section by Perkins et al. (2012), Cuitíño et al. (2015, 2019) imply that the base of the Santa Cruz Formation is at ca. 19 Ma. Blisniuk et al. (2005) reported 40Ar/39Ar ages for six tuffs and stable carbon (δ13C) isotope ratios of ~250 paleosol carbonate samples of similar overlapping ages. We evaluated the age and its uncertainty for each carbonate nodule based on its stratigraphic position. These uncertainties are large, typically ±1 Ma. Given that changes in isotope composition are commonly used as a proxy for ecological, climatological, and tectonic change (Koch, 1998; Poage and Chamberlain, 2001), it is extremely important to incorporate these significant age uncertainties during the transformation from the spatial (stratigraphic height) domain to the time series, and the subsequent analysis and correlation of these isotopic records to global change (Blaauw et al., 2007; Parnell et al., 2008).

Discrete stratigraphic proxy record samples (e.g., stable isotopes, palynofloras, phytolith assemblages) are commonly transformed into a continuous temporal record through the use of age models and smoothing and interpolation functions. Many age-depth transformations are deterministic in nature, while most common smoothing functions (moving averages, polynomials, splines) assume that errors are either nonexistent or normally distributed. Both of these assumptions are inconsistent with our models’ prediction of age for each proxy record (carbonate nodules). Each age-depth model consists of many possible sample chronologies (e.g., Fig. 2). By using these probabilistic chronologies to predict the age of the carbonate nodules, the age of each nodule is allowed to vary while still preserving the superpositional relationships among nodules. This is accomplished using the following steps:

1. Use age-depths model results to choose a set of ages for each proxy record based on its stratigraphic position.
2. Apply an appropriate smoothing function (in this case a moving average) to the proxy data (in this case carbon isotopes) given the chosen set of ages and store the results.
3. Repeat many times and calculate summary statistics (e.g., median, HDI) over all smoothed proxy records.

A moving average through the Lago Posadas carbon isotope data (from Blisniuk et al. 2005) versus stratigraphic position (Fig. 7B) illustrates the limitations of fitting a single smoothing function to a data set. In stratigraphic regions with low data density (e.g., ~200 and 290 m), the single moving average model shows significant spikes and wiggles in isotope composition. These abrupt variations include a rapid increase at 200–215 m that Blisniuk et al. (2005) interpreted as beginning at ca. 16.5 Ma based upon a deterministic age model. The authors attributed this shift to an increase aridity driven by a pulse of Andean uplift at 16.5 Ma. However, when age model uncertainties are considered it becomes clear that where there is low data density in a stratigraphic context, there are many other samples of similar overlapping ages (Fig. 7C), which must influence and reallocate the probability of the proxy value in the temporal domain.

While the single moving average model suggests rapid shifts in δ13C in the stratigraphic reference frame, propagated age model uncertainties instead suggest that in a rigorous probabilistic temporal reference frame, δ13C values possibly began increasing ~0.6 m.y. earlier at 17.1 Ma, and continued gradually until at least 16 Ma, with δ13C values then remaining essentially unchanged until the end of the record.

The use of a probabilistic age-depth model and the propagation of model uncertainties therefore has implications for both the timing and rate of isotopic change. The moving average model originally reported by Blisniuk et al. (2005) implies that the initial increase in δ13C values at 200–215 m could have occurred rapidly over as little as ~0.06 m.y., whereas our re-evaluation permits a much more gradual increase extending over ~1 m.y. Significantly, an increase in δ13C values at the revised age of ca. 17 Ma corresponds to the onset of the mid-Miocene climatic optimum, a period of overall increased global temperatures (Holbourn et al., 2015; Zachos et al., 2001). Global climate change may therefore provide a plausible alternative explanation for the vegetation shifts that drove changes to δ13C values. Finally, converting stratigraphic position to age also simplifies and lends rigor to comparisons of proxy records between localities that lack correlative stratigraphic features. This stratigraphic to temporal transformation is vital for terrestrial sequences sensitive to hiatuses and rapid changes in depositional environment and rate.

CONCLUSIONS

While Bayesian age-depth modeling is commonly used with Quaternary radiocarbon ages, existing models have seen only limited deep-time use. We have demonstrated the features of a modified Bayesian age-depth model amenable to deep-time scenarios using new U-Pb ages of zircon and existing 40Ar/39Ar ages from the Santa Cruz Formation. Proposed tuff correlations link exposures at Killik Aike Norte to the upper section at Cañadón de las Vacas and Rincón de Buque, providing a new correlation among these localities.

We view our model results as largely consistent with both our U-Pb and existing 40Ar/39Ar data for the Santa Cruz Formation, requiring only small adjustments to ages. While these shifts are small, we view model results as the most robust estimate of age. In many cases the model improves uncertainties of imprecise data (i.e., CO2 tuffs). The greatest improvements occur when closely spaced tuffs are dated, further showing the value of dating several samples through a stratigraphic section. Allowing the model to explore the full variance present in magmatic zircon...
Age modeling in deep time

Figure 7. (A) Age-depth model for Lago Posadas, Argentina. Pink points and error bars indicate the median and 95% HDI model ages for paleosol carbonate nodules. (B) Plot of the carbon isotope composition of paleosol carbonates versus stratigraphic position, with a weighted moving average with a 5 m window size. (C) Plot of carbonate carbon isotope compositions versus age. Error bars indicate the 95% high density interval (HDI) of age for each point as in A. Black line is the median of 100,000 Gaussian weighted moving averages (0.2 Ma window size), where the age of each point was allowed to vary probabilistically based on age model results. Ninety-five percent of the moving average models fall within the shaded pink area.

TABLE 3. SUMMARY STATISTICS OF THE LIKELIHOOD AND POSTERIOR AGE FOR EACH TUFF FROM THE LAGO POSADAS SECTION, SANTA CRUZ FORMATION, ARGENTINA

<table>
<thead>
<tr>
<th>Sample</th>
<th>Stratigraphic position (m)</th>
<th>Weighted mean likelihood</th>
<th>Weighted mean (Ma)</th>
<th>95% HDI model age (Ma)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LP-1</td>
<td>504.5</td>
<td>14.24 ± 1.56</td>
<td>13.64 ± 1.14/1.35</td>
<td></td>
</tr>
<tr>
<td>LP-331</td>
<td>331.5</td>
<td>15.61 ± 0.82</td>
<td>15.46 ± 0.59/0.68</td>
<td></td>
</tr>
<tr>
<td>LP-251</td>
<td>251.7</td>
<td>16.56 ± 0.50</td>
<td>16.49 ± 0.39/0.45</td>
<td></td>
</tr>
<tr>
<td>LP-181</td>
<td>181.2</td>
<td>16.82 ± 1.02</td>
<td>17.29 ± 0.67/0.61</td>
<td></td>
</tr>
<tr>
<td>LP-58</td>
<td>58.8</td>
<td>18.27 ± 0.62</td>
<td>18.45 ± 0.59/0.60</td>
<td></td>
</tr>
</tbody>
</table>

Notes: Weighted mean ages uncertainties are reported as a mean ±2σ; all other ages are reported as a median and 95% highest density interval (HDI). Weighted mean ages were originally reported in Blišniuk et al. (2005) and recalibrated by Perkins et al. (2012).

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De Vleeschouwer, D., and Parrish, A.C., 2014, Reanalysis of carbon isotope data from the Lago Posadas paleosol record could for example arise from cyclic climatic forcing, it could warrant by strong evidence. In the second case, using model uncertainties to inform the interpretation of proxy record data also shows promise. Reanalysis of carbon isotope data from the Lago Posadas paleosol record (Blišniuk et al. 2005) with age model uncertainty reveals a gradual increase in δ13C values from ca. 17–16 Ma, suggesting the probability of both an earlier initiation and slower change than originally reported. We view this as a more conservative and robust interpretation of the proxy record, which highlights the general need (Blaauw et al., 2018) for the collection of stratigraphically dense, high-precision geochronologic data cast within a robust Bayesian age model framework.