A reporting protocol for thermochronologic modeling illustrated with data from the Grand Canyon

Rebecca M. Flowers^{1*}, Kenneth A. Farley², Richard A. Ketcham³

¹ *Department of Geological Sciences, University of Colorado, Boulder, Colorado, USA*

² *Division of Geological and Planetary Sciences, Pasadena, California, USA*

³ *Jackson School of Geosciences, University of Texas, Austin, Texas, USA*

** To whom correspondence should be addressed:*

Email: rebecca.flowers@colorado.edu, Phone: 303-492-5135

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Abstract

Apatite (U-Th)/He and fission-track dates, as well as $^4\text{He}/^3\text{He}$ and fission-track length data, provide rich thermal history information. However, numerous choices and assumptions are required on the long road from raw data and observations to potentially complex geologic interpretations. This paper outlines a conceptual framework for this path, with the aim of promoting a broader understanding of how thermochronologic conclusions are derived. The tiered structure consists of thermal history model inputs at Level 1, thermal history model outputs at Level 2, and geologic interpretations at Level 3. Because inverse thermal history modeling is at the heart of converting thermochronologic data to interpretation, for others to evaluate and reproduce conclusions derived from thermochronologic results it is necessary to publish all data required for modeling, report all model inputs, and clearly and completely depict model outputs. Here we suggest a generalized template for a model input table with which to arrange, report and explain the choice of inputs to thermal history models. Model inputs include the thermochronologic data, additional geologic information, and system- and model-specific parameters. As an

example we show how the origin of discrepant thermochronologic interpretations in the Grand Canyon can be better understood by using this disciplined approach.

1. Introduction

Low temperature thermochronology has advanced rapidly over the last two decades. The combination of apatite (U-Th)/He (AHe) and $^4\text{He}/^3\text{He}$ dating, along with apatite fission-track (AFT) dates and fission-track length (FTL) distributions, together characterize the migration of a rock sample through temperatures from ~120-30°C. The uniquely low temperatures accessible through these systems has led to an abundance of studies documenting the cooling and heating of rocks in the upper few kilometers of the Earth's crust, as well as established a quickly expanding user base of these techniques (see Reiners & Ehlers, 2005). The wealth of thermal information available from these combined systems, and the number and variety of measurements and geologic observations that are brought to bear in a given study, increasingly demand sophisticated models to derive accurate and defensible geologic interpretations. However, the path from observation to geologic interpretation is long, and in many studies it is difficult to understand all the steps, choices, and assumptions made along the way. As a result, it is frequently challenging to assess an interpretation's robustness, understand why and how it was developed, and determine how it can be refined or tested.

In this paper we propose a protocol for organizing and reporting the information necessary for thermochronologic modeling. Our objective is to enhance understanding of how thermochronologic interpretations are obtained. The concepts here have strong synergy with ongoing efforts to archive geochronologic measurements, but are focused at

a higher interpretive level. The suggested template can not only help guide new users of thermochronologic methods in deriving robust interpretations of their own datasets, but also, if adopted, would help clarify the origin of interpretations in specific studies and better focus future work. Our interest in these issues first arose from recent studies that yield disputed interpretations of the antiquity of the Grand Canyon (Flowers & Farley, 2012, 2013; Karlstrom et al., 2014). The quantity and diversity of observations brought to bear on this problem, and the complexity of the modeling involved, illustrate how difficult it can be to identify the source of contrasting conclusions. We first outline a conceptual structure for the path from data to geologic interpretation, then discuss the building blocks of this hierarchy by reviewing the methodologies involved, propose a generalized model input reporting protocol, and provide an illustration using the Grand Canyon.

2. Data Levels: From Data to Geologic Interpretation

Figure 1 offers a structure by which to construct a rigorous path of argument extending from thermochronologic observations to sophisticated geologic interpretations. We adopt a scheme in which there are multiple data levels, advancing from rawer data and simpler observations to data products that include increasing interpretation by linking elements derived from the previous level. By defining all elements within this tiered framework it becomes possible to analyze the argumentation, identify the source of differences among competing interpretations arising from the same or related data, and investigate how each element contributes to the interpretation. This interpretational hierarchy is adapted from the data levels used by NASA and EarthScope (e.g., Gurnis et

al., 2012), although we do not employ their strict definitions of unprocessed and derived data at different levels. Rather we modify this approach for our context in the manner described below.

Level 1 of the framework consists of model input, which can be subdivided into three broad categories: thermochronologic data, additional geologic information, and system-specific and model-specific parameters. Broadly speaking, *thermochronologic data* can be seen as consisting of the totality of the measurements, from isotopic and elemental compositions to fission-track lengths and step-heating spectra, and documentation of how they were made and processed into derived quantities such as dates. This category may be taken to correspond to the information that would be entered into a database of geochemical and/or geochronologic data resulting from community efforts for a given technique. In addition, this category includes which measurements are selected and/or combined for including in the model. *Additional geologic information* consists of independent data that result in direct model input, such as depositional age and temperature, and non-modeled ages such as zircon U/Pb. This category also may include explicit assumptions being made and hypotheses being tested, such as the timing of peak heating. Finally, *system- and model-specific parameters* include the kinetic models used for thermal history modeling, the modeling code, and input specific to that modeling code such as statistical fitting criteria or algorithm parameters. Note that many of these model inputs are derived from still rawer data using basic assumptions and physical models (examples of inputs to He and AFT data in Figure 1).

Level 2 of the framework includes the output (allowed tT paths) of an inversion model developed with and honoring the Level 1 inputs. Thus each Level 1 element can be

viewed as a building block for a Level 2 result – by linking together different Level 1 elements, different Level 2 results may be obtained. At Level 2 the allowed tT paths can then be horizontally integrated with additional geologic observations and assumptions to achieve the geologic interpretations at Level 3.

In the next section we provide a brief overview of the relevant methods. We confine our discussion here to apatite, as the most-studied and best-characterized mineral of both the (U-Th)/He and fission-track systems. Extensive reviews of both AHe and AFT exist (e.g., Donelick et al., 2005; Reiners and Ehlers, 2005); our goal here is only to motivate and explain aspects of the methods that are critical to accurate thermal history modeling and thus are important Level 1 elements.

3. Underpinnings of Low Temperature Thermochronology

3.1 The apatite (U-Th)/He system

AHe chronometry is based on α decay of U, Th, and Sm. Over geologic timescales He is strongly retained in apatite at Earth surface conditions, but is rapidly lost via thermally-activated volume diffusion at temperatures above $\sim 100^\circ\text{C}$. A reference point for understanding cooling dates is provided by the closure temperature (Dodson, 1973), which for the AHe system varies from ~ 55 to $>100^\circ\text{C}$ depending on radiation damage, grain size, and cooling rate. AHe dates are derived from measurements of the parent and daughter abundances in an entire crystal. The apatite $^4\text{He}/^3\text{He}$ method is a variant in which the ^4He concentration profile is characterized. The utility of this method is that the concentration profile documents the degree of diffusional rounding of ^4He in the sample, which is sensitive to the apatite's temperature history (Shuster and Farley,

2003). An apatite's bulk He concentration is simply the integral of this profile over the entire crystal. Thus bulk dates and $^4\text{He}/^3\text{He}$ spectra are not completely independent observations – rather the $^4\text{He}/^3\text{He}$ method provides insight into how the bulk date was developed.

Alpha particles travel $\sim 20\ \mu\text{m}$ after parent decay, and this distance is often a significant fraction of the size of an apatite crystal. When an apatite's surroundings have negligible parent concentrations compared to the apatite itself, the net result is α -ejection. Given a crystal's size and geometry, this effect can be modeled (e.g., Farley et al., 1996; Hourigan et al., 2005; Ketcham et al., 2011). Most AHe dates are corrected for this effect assuming a hexagonal prism geometry. However, the accuracy of this correction is increasingly suspect as grain size decreases and the correction's magnitude increases. Regardless of whether a correction is made, α -ejection modifies the shape of the ^4He profile, and thus affects the diffusional loss rate. In some cases the assumption of negligible parent concentration surrounding an apatite is violated, leading to He implantation and erroneously old and often highly scattered He dates. Because analyzed apatites carry no record of their neighborhood, He dates cannot generally be corrected for this effect (Murray et al., 2014; Spiegel et al., 2009).

Zonation of parent nuclides is an additional consideration. Zonation matters because it affects the α -ejection correction, modifies the ^4He concentration profile on which diffusion acts and which the $^4\text{He}/^3\text{He}$ method documents, and likely contributes, via heterogeneous radiation damage accumulation, to variation in diffusion kinetics within a grain (Farley et al., 2011). In some cases, particularly for studies using the $^4\text{He}/^3\text{He}$ method, parent nuclide distribution is measured using laser ablation ICPMS

(Farley et al., 2011; Johnstone et al., 2013). The measured distribution must be converted into an appropriate representation of the distribution within the three-dimensional grain (e.g., Farley et al., 2011). Since the $^4\text{He}/^3\text{He}$ spectrum is very sensitive to zonation (Farley et al., 2010), apatites with extreme zonation (which is difficult to constrain by limited LA-ICPMS data), are inappropriate for $^4\text{He}/^3\text{He}$ work. He dates are not strongly affected by typical apatite zonation magnitudes (Ault and Flowers, 2012). In the absence of a measured parent nuclide distribution, analysts commonly assume homogeneity.

Ideally, apatite grains selected for AHe dating are complete and euhedral, but in practice such grains may not be available, and rounded grains or fragments are used. This can introduce additional uncertainty that is difficult to quantify due to breakage effects on the diffusion domain size and the α -ejection correction, especially if the timing of abrasion or breakage is unknown (Brown et al., 2013).

Acquisition of an AHe date involves selection of individual inclusion-free apatite crystals, crystal dimension measurement, He degassing and analysis, apatite dissolution, and U, Th, and Sm analysis by ICPMS. The grain dimensions constrain the size of the diffusion domain (usually converted into an equivalent spherical radius) and the magnitude of the α -ejection correction. Most labs report single-grain AHe dates with errors that include the propagated uncertainties on the parent and daughter abundances (typically a few %), but may or may not include the uncertainty in the α -ejection correction, and cannot include effects that are unmeasured, unknown, or unquantifiable, such as implantation, zoning or fragmentation. Some labs instead report a blanket uncertainty based on repeated measurements of standards. It is frequently useful to combine parent nuclide abundances into a single quantity that approximates the total α -

production, which is a proxy for the amount of radiation damage accumulated in an apatite not experiencing annealing. This quantity is known as “effective uranium” (eU, where $eU = U + 0.235Th$ in ppm; Sm contributes too little to require inclusion in this approximation).

The $^4He/^3He$ method is analytically complex and therefore less commonly applied. In this method, ideally whole, euhedral apatites are irradiated with energetic protons to create a uniform distribution of 3He via spallation, and then subjected to a step-heating experiment in which the evolved $^4He/^3He$ ratio is measured. The $^4He/^3He$ spectrum (i.e., the measured ratio as a function of the cumulative amount of 3He evolved) is related to the 4He concentration profile within the grain. The $^4He/^3He$ spectrum can be converted into an age spectrum by normalizing to the 4He concentration profile produced by α -ejection alone, and to the sample's AHe date (Shuster and Farley, 2005).

Knowledge of He diffusion kinetics is critical to the interpretation of AHe data. While early studies drew heavily on a He diffusion kinetic model derived from laboratory experiments on the Durango fluorapatite (“Durango model”, Farley, 2000), it is now known that radiation damage strongly influences apatite He diffusivity (Shuster et al., 2006). This effect is manifested as date-eU correlations in apatite suites that experienced especially susceptible thermal histories (e.g., Flowers et al., 2007). The radiation damage accumulation and annealing model (RDAAM) accounts for the evolution of apatite He retentivity during the addition and elimination of α -damage (Flowers et al., 2009). A similar model was proposed by Gautheron et al. (2009). Experiments suggest that fission damage annealing is a reasonably good proxy for the annealing of damage that influences

He diffusion (Shuster and Farley, 2009), so the RDAAM uses a fission track annealing model to follow radiation damage elimination (Flowers et al., 2009; see also section 3.2).

Helium diffusivity will vary among apatites in a rock due to variations in radiation damage and grain size. Similarly, diffusivity varies over the history of the apatite crystal owing to accumulation and annealing of radiation damage. Thus for a rock that has spent time in the region of partial He retention (90-30°C), He dates may vary from crystal to crystal well outside of an individual date's analytical precision. Provided the date variability can be related to causative factors (grain size, eU, annealing properties, crystal fragmentation), this variability enhances the thermochronometric value of a suite of dates from the same rock (e.g., Brown et al., 2013; Flowers and Kelley, 2011). However, if date variability is uncorrelated with such factors, interpretation is problematic and may lead to failure of inverse thermal history models to yield any acceptable tT paths, or require the analyst to make subjective choices concerning how to use over-dispersed data, whether by some kind of averaging or choosing which grains to include and exclude. Thus great care must be exercised when modeling samples with inexplicably large variability in AHe dates.

3.2 The apatite fission-track system

Unique among naturally occurring isotopes, ^{238}U undergoes spontaneous fission at a geologically significant rate. The high energy of this decay is carried off as motion of a pair of fission daughters whose passage through crystals is recorded in the form of a damage track. Given a fission decay constant for ^{238}U , the U concentration, and the density of fission tracks (FTs), an accumulation time or date can be obtained. In the case

of apatite, FTs can be revealed for microscopic examination and counting through acid etching. Apatite FTs experience time and temperature-dependent annealing, so an AFT date is, like a (U-Th)/He date, a reflection of the apatite's tT path. The AFT system is especially sensitive to temperatures in the range ~60-110°C (Gleadow and Duddy, 1981), with possible resolution of still lower temperatures (Ketcham et al., 2009), and fluorapatite is typically assigned a closure temperature of ~100°C .

An AFT date is obtained by counting the abundance of spontaneous fission tracks revealed in an acid-etched polished surface, and comparing that abundance with a U concentration determined either by counting of ²³⁵U fission tracks induced by neutron activation, or by using LA-ICPMS. Due to historic and in some cases ongoing uncertainties with a number of relevant quantities, including the fission decay constant, reactor neutron fluence measurement, and track revelation and measurement efficiency and bias, most labs calculate dates based on age standards using the zeta method (Hurford, 1990; Donelick et al., 2005), although some groups endorse absolute age determination (e.g., Enkelmann et al., 2005). The number of spontaneous tracks exposed in a polished grain surface is typically small, leading to large statistical variations between grains of the same age. "Pooled" AFT dates for a sample are obtained by simply combining observations from multiple individual apatite grains. When the date dispersion among a population of grains from a single sample exceeds that expected from Poissonian statistics applied to the number of tracks counted, it is common to report the geometric mean of the dates, called the central age (Galbraith and Laslett, 1993).

Fission-track length (FTL) data are obtained from confined horizontal tracks, in which etchant has traveled into the grain via some pathway (typically a fission track or

cleavage plane) and intersected and etched out an interior track with both ends enclosed in the solid. Revelation of FTL's can be enhanced by bombarding the polished grain surface prior to etching with ^{252}Cf fission fragments (Donelick and Miller, 1991) or heavy ions (Jonckheere et al., 2007). Because apatite is anisotropic with respect to both etching and annealing, the angle of each confined track to the crystallographic **c** axis is also usually measured. FTL data may be normalized for anisotropy using **c**-axis projection, which converts each track to an estimated **c**-axis-parallel equivalent (Donelick et al., 1999). Because they incorporate additional information, projected track lengths are generally more precise indicators of thermal history than unprojected lengths (R. a. Ketcham et al., 2007). FTL data is also prone to biases and variation among analysts, and it has recently been proposed that calibration against length standards and **c**-axis projection should be used to improve inter-laboratory reproducibility (Ketcham et al., 2015)

The annealing process involves progressive shortening of the FT from an initial length of 16-18 μm until it ultimately disappears. Each track within an apatite has experienced the temperature history and any associated track shortening from the time of the track's formation until the present. Thus, the FTL distribution provides additional information on the sample's **tT** path. The complementarity between an AFT date and its associated FTL distribution is analogous to that of an AHe date and its $^4\text{He}/^3\text{He}$ spectrum. FTL distributions are commonly reported either as a table of measured lengths, or as a mean track length and standard deviation. For **tT** modeling the complete distribution, rather than a statistical abstraction, is essential.

Laboratory investigation of annealing rates contribute to an understanding of annealing, which in turn provides a foundation for kinetic models used to constrain a tT path from AFT dates and FTL distributions. In addition to primary control by temperature, the annealing rate and thus closure temperature of AFTs is affected by chemistry, in particular the relative abundance of Cl (and possibly OH) in the anion site, as well as some cation substitutions (e.g., Carlson et al., 1999; Green et al., 1986). Thus reliable interpretation of AFT data requires information about apatite annealing kinetics. Annealing kinetics can be estimated based on a single compositional variable (i.e. Cl content), a multi-compositional approach (r_{mro} ; Ketcham et al., 1999), or solubility, which reflects chemistry and is conveniently measured as the diameter of etch figures parallel to the **c** axis (D_{par} ; Burtner et al., 1994).

Ideally the kinetic parameter should be measured on every apatite grain used in age and length measurements, and, analogously to date-eU correlations for AHe, kinetic effects can be inspected for by plotting single-grain dates and track lengths against the kinetic parameter. If correlations are found, it is often possible to group measurements into statistically coherent populations with distinct annealing properties that can be modeled in tandem. Although this step is frequently omitted during interpretation and modeling, doing so is hazardous, as mixed populations of ages and lengths may lead to nonsensical results if interpreted with the assumption that they are kinetically homogeneous. Although several apatite fission-track annealing models are available for interpreting FTLs and AFT dates (e.g., Crowley et al., 1991; Laslett et al., 1987), only the more recent ones incorporate compositional and track-angle information (Ketcham et al., 1999; Ketcham et al., 2007b).

4. Thermal history modeling and its documentation

4.1. Model inputs, outputs, and interpretation

Although AHe and AFT results are reported as dates, these quantities typically do not indicate the date of a geologic event or even cooling through the closure temperature. Instead they are single-valued quantities that capture the apatite's integrated thermal history since the onset of He retention and/or radiation damage accumulation. Inversion models (e.g., Ketcham, 2005) are used to constrain this thermal history, and so are at the core of making geologic interpretations from thermochronologic measurements. The inversion models take kinetic models that describe how the AHe and AFT systems respond as a function of temperature and time, and yield tT paths consistent with thermochronometric observations and a priori geologic constraints.

A diversity of tT paths can yield the same AHe or AFT date, so a unique path generally cannot be determined. Combining multiple approaches (AHe, AFT, $^4\text{He}/^3\text{He}$, FTL distributions) on a single sample can reduce this non-uniqueness. Similarly, samples strategically drawn from the landscape or down a borehole can restrict feasible tT paths. For example, elevation transects are commonly employed because the paths must be internally consistent across the sample suite (e.g., Gallagher, 2012). Geologic considerations, such as igneous crystallization ages, the age of a faulted volcanic unit, or the age of an unconformity, can also eliminate possible paths. Geologic constraints can strongly bias inversion model output, so these must be defined and justified with appropriate rigor.

Even with the numerous constraints provided by multiple systems and samples, inversion model outputs are typically a swath of acceptable tT paths. The question of how one defines acceptability given diverse data types and sometimes poorly characterized uncertainties is a complex topic that we do not address here. Several contributions discuss the rationale for the approaches employed by HeFTy and QTQt, the two most widely used inverse modeling programs for thermochronologic data (Gallagher, 2012, 1995; Ketcham, 2005; Vermeesch and Tian, 2014).

A key point of this paper is that in addition to the target dates, $^4\text{He}/^3\text{He}$ spectra, and FTL distributions, these models require specification of a large number of additional quantities. These include, for example, the ancillary information required for kinetic modeling (Sections 3.1 and 3.2, Figure 1) as well as specification of initial and final temperature conditions, the character of the allowed tT paths, the statistical fitting thresholds applied, and any imposed geologic constraints. Without documentation of all of this input information, the modeling results cannot readily be reproduced.

Equally important is the clear, complete, and accurate representation of the thermal history model outputs. Within the swath of acceptable fits, there is no statistical justification to prefer the "best fit" path over the others. Summary paths, such as a weighted mean (Ketcham 2005) or Bayesian "expected model" (Gallagher 2012), can sometimes be helpful when comparing multiple model results, but their use in this manner can also be perilous if it's not made clear that they are simplifications of a much wider range of acceptable solutions. Some characterization of the full suite of statistically valid tT paths should be displayed on the tT result plot whenever possible, and must be made easily available elsewhere when not, because its omission makes it impossible to

evaluate the actual restrictiveness of the model output. The imposed tT constraints should also be shown, because without them one cannot assess the extent to which these defined constraints or the thermochronologic data determined the model results.

When interpreting and discussing the model outputs, it is important to distinguish between results that *require*, *exclude*, or are *consistent with* a particular interpretation (see example in section 5.3). Geologic conclusions based on these results then entail additional assumptions about geotherms, surface temperatures, and other factors.

4.2. The thermal history model input table

Level 1 of the interpretational framework (Fig. 1) encompasses the totality of the building blocks from which the Level 2 results – the thermal history model outputs - are derived. We suggest that use of a model input table with which to clearly define, rigorously explain, and, if necessary, provide references for, each and every one of the Level 1 inputs to thermal history models would help clarify how thermochronologic conclusions are derived in individual studies. Table 1 is an example, which subdivides the input parameters into 3 types: thermochronologic data, additional geologic information, and system- and model-specific parameters.

The thermochronologic data include a list of all thermochronologic information constraining a given model, as well as where the data needed to reproduce the model were published if not reported in the same paper. This section additionally notes the uncertainties applied, catalogues any ancillary data used or assumed in the thermal history simulations (e.g., eU zonation or weight % Cl), and explains how the data were treated - for example, whether and how data from multiple analyses or rocks were

combined. The second type of model input includes all other constraints imposed on the tT paths, which are typically derived from geologic information. Not only should the imposed tT constraint be listed, but the geologic rationale for it articulated, and the relevant reference provided. Model-specific parameters compose the final suite of Level 1 building blocks. We include here the kinetic models used, the statistical fitting criteria applied for defining the tT paths allowed by the data, the modeling code employed, and details such as the number of thermal histories evaluated.

The structure of the model input table underscores that by linking together different Level 1 elements, different Level 2 tT outputs may be obtained. For example, as further analyses are undertaken, the number of available chronometric elements may increase. Or a new or different diffusion kinetic model may replace the one originally chosen. Similarly, by excluding or modifying a specific Level 1 element, it becomes possible to assess which element drives specific aspects of the Level 2 results. We next illustrate the value of such a model input table using as an example a thermochronologic dataset from the Grand Canyon.

5. An Illustration of the Model Input Table using the Westernmost Grand Canyon

The age of the Grand Canyon has long puzzled geologists. The prevailing model has held that the entire canyon was carved after 6 Ma (e.g., Karlstrom et al., 2008), but recent thermochronologic datasets have reinvigorated discussion about the canyon's antiquity. AHe and $^4\text{He}/^3\text{He}$ data were used to argue for a multiphase history in which the modern gorge of the western (but not the eastern) canyon was partially excavated by ~70 Ma (Flowers and Farley, 2012; Wernicke, 2011). Several ensuing studies used additional

thermochronologic data to similarly conclude that the canyon's history was more complex than simple post-6 Ma incision (Lee et al., 2013) with one segment as old as 65 Ma (Karlstrom et al., 2014). Thus, recent debate has shifted to focus on which reaches of the Grand Canyon are old, and when and how different paleocanyon segments became linked. A point of disagreement is whether the westernmost Grand Canyon (WGC; Fig. 2A, 2B) is ancient (partially carved by 70 Ma; Flowers and Farley, 2012; Wernicke, 2011) or young (incised entirely after 6 Ma; Karlstrom et al., 2014). The dataset for this canyon segment includes AHe, $^4\text{He}/^3\text{He}$, AFT, and FTL data for multiple samples. Our objective here is not to address the canyon's age, but rather to show how a rigorous reporting protocol, as well as complete model output representation, can facilitate understanding of thermochronologically-derived conclusions.

5.1. Thermochronologic data

The thermochronologic data currently available for the WGC are shown in Figure 2B. All samples are Proterozoic basement from an ~56 km stretch of the canyon bottom. The data include AHe results for seven samples, four of which have U-Th zonation data (Flowers and Farley, 2012; Flowers et al., 2008; Lee et al., 2013). Fourteen apatite $^4\text{He}/^3\text{He}$ spectra are available for two of them (Flowers and Farley, 2012). AFT dates are reported for 4 samples (Kelley et al., 2001; Lee et al., 2013). Three of these have FTL information and 3 have coexisting AHe data.

The data are plotted versus River Mile in Figures 2C, 2E, and 2F, measured by convention from Lee's Ferry (RM 0). Six of the samples with AHe data include 29 single-grain analyses generated independently in two labs, and yield mean sample dates from

70-89 Ma and within-sample reproducibilities of 4-13% (red symbols, Fig. 2C). This age clustering and level of reproducibility supports the reliability of the dataset. In contrast, a seventh rock (01GC86) with 43% dispersion (1σ) for three AHe dates, coupled with its much younger mean date of 50 Ma, suggest a problematic sample (blue symbol, Fig. 2C). As noted in section 3.1, AHe samples like this one with extreme date scatter for which no kinetic control has been identified are generally inappropriate for inversion modeling.

Of the available $^4\text{He}/^3\text{He}$ spectra, only the CP06-69 data are adequate for modeling (Fig. 2D). The three replicate spectra for this sample are similar, although the third grain (not shown in Fig. 2D) included an anomalous final step in the spectrum. This sample's apatites have similar and fairly muted U-Th zoning patterns. In contrast, the eleven $^4\text{He}/^3\text{He}$ spectra from sample GC863 are highly variable, likely a consequence of the observed extreme and variable U-Th zonation. As discussed in Section 3.1, such apatites will have $^4\text{He}/^3\text{He}$ spectra dominated by the comparatively uncertain parent nuclide distribution rather than by diffusion, and so are inappropriate for tT modeling.

The available AFT dates range from 75 ± 5 Ma to 63 ± 4 Ma, reported as the central age and 1σ S.E. of the pooled dates (Fig. 2E; Kelley et al., 2001; Lee et al., 2013). FTL distributions of the three samples are distinct, varying from 14.0 ± 0.4 μm to 12.1 ± 0.4 μm (mean and 1σ S.E.). Individual grain dates, FTLs, and kinetic parameters were not published, precluding others from modeling these data and rigorously evaluating the conclusions derived from them.

5.2. WGC model input tables (Level 1 documentation)

To illuminate how discrepant conclusions were reached about the age (70 Ma vs. <6 Ma) of the WGC from the above dataset, we assembled the model input tables for the relevant thermal history simulations using the information provided in Flowers and Farley (2012, 2013) and Karlstrom et al. (2014). All simulations used the HeFTy software program. For simplicity we label the simulations from #1-6 in the tables, figures, and text.

Table 2 is the model input table for the 3 key simulations of Flowers and Farley (2012, 2013) from which their ancient WGC interpretation was derived. Their approach was to simultaneously satisfy all Level 1 thermochronologic data from the WGC, which assumes that this suite of canyon bottom samples experienced the same thermal history. Simulation #1 included duplicate $^4\text{He}/^3\text{He}$ spectra for CP06-69, as well as all 4 then available AHe samples and their U-Th zonation data (Table 2). It was impossible to include the only then available WGC AFT data (sample 98GC38) in this inverse model, because the individual grain dates and FTLs were unpublished (Kelley et al., 2001; see section 5.1). However, the Cretaceous central age and long FTLs reported for this sample indicated complete annealing of FTs at peak temperature, providing a zero radiation damage, zero He date initial condition for modeling. Consequently, the inversion model was initiated at 100-80 Ma at temperatures $\geq 110^\circ\text{C}$ to honor this AFT constraint. The only other tT constraint imposed was the requirement to reach modern surface temperatures of 20-25 $^\circ\text{C}$ by present day. Two other simulation variants included AHe data for a single sample only (sim #2), or incorporated the $^4\text{He}/^3\text{He}$ spectrum for a third apatite (spectrum b from CP06-69 with an anomalous final step; sim #3; Flowers and

Farley, 2013). These latter simulations were considered consistency checks because they did not seek to honor all available data simultaneously.

Lee et al. (2013) subsequently reported new AHe and AFT data for 3 WGC samples, but performed a tT simulation for only one of them. Karlstrom et al. (2014) carried out 3 thermal history models, one for each of these new samples. Unfortunately, the AFT single grain dates and FTLs necessary for others to reproduce these simulation results and generate additional models remain unpublished. The Karlstrom et al. (2014) models, which we here call simulations 4, 5, and 6, differ from those of Flowers and Farley (2012, 2013) in modeling different samples, using AFT dates and FTLs as Level 1 observations, not using $^4\text{He}/^3\text{He}$ data, and using different tT constraints that limit peak temperatures to $\leq 110^\circ\text{C}$. Importantly, Karlstrom et al. (2014) treat each sample separately rather than simultaneously satisfying all data, therefore relaxing the requirement that all WGC samples have the same thermal history. Simulation #4 models the AHe and AFT dates for sample 01GC89 (no FTL data are available). Simulation #5 simulates the AHe, AFT, and FTL data for sample 01GC87. Simulation #6 uses the problematic AHe data from sample 01GC86 (Fig. 2C, blue symbols).

5.3. Model outputs and their interpretation (Levels 2 and 3)

The distinct conclusions regarding when the WGC was initially carved arise from the differing tT model results in Figure 3. Results for simulations #1-3 from Flowers and Farley (2012, 2013) are displayed as individual tT paths (Fig. 3A-C). The key result is that all thermal histories require cooling to $<30^\circ\text{C}$ by 70 Ma. This result is supported by both simulation #1 that honored multiple observations simultaneously (Fig. 3A; Flowers

and Farley, 2012), as well as the consistency checks provided by simulating AHe and $^4\text{He}/^3\text{He}$ data for a single sample only (sim #2, Fig. 3B) and by including the $^4\text{He}/^3\text{He}$ spectrum for a third apatite (sim #3, Fig. 3C; Flowers and Farley, 2013). This outcome is consistent with the previously published simulation result for what was then the only available westernmost canyon AFT data (sample 98GC38), which allowed for (but did not require) cooling to 30 °C by ca. 65 Ma (Fig. 3D, from Kelley et al., 2001, tT path output shown as fields). Based on this internal consistency, Flowers and Farley (2012, 2013) concluded that rocks along the bottom of the WGC segment had cooled to <30 °C by 70 Ma. They then argued that 20-25°C/km and 20-25°C are appropriate geotherm and surface temperature estimates, respectively, and assuming these values concluded that the ~1000 m deep modern gorge of the WGC was partially carved by 70 Ma. They also contended that the predictions of a thermal history associated with entirely post-6 Ma incision are inconsistent with the AHe and $^4\text{He}/^3\text{He}$ data (Flowers and Farley, 2012).

The key figure from Karlstrom et al. (2014) representing their model outputs is shown in Figure 3E. This plot depicts seven different tT model results, including those for simulations #4-6 discussed in the previous section, results for two additional samples not from the WGC, the AFT model result of Kelley et al. (2001), and the swath of results from simulation #3 of Flowers and Farley (2013). For most of these models Karlstrom et al. (2014) chose to depict only a single path (unspecified, but most likely the weighted mean of acceptable paths), rather than the full suite of statistically valid results. They also do not show the tT constraints imposed on the models here. Karlstrom et al. (2014) used this figure to support their conclusion of variable thermal histories along the WGC and young (<6 Ma) canyon incision, because at face value Figure 3D suggests rather extreme

variations in tT paths, with many samples seemingly supporting temperatures $>30^{\circ}\text{C}$ until well after 70 Ma. However, by referring to the model input table (Table 3), as well as to the full output plots for several models, we can assess why this variability exists and whether it is required. Two of the model results depicted on Figure 3E (dark blue curves) are for two samples located ~ 60 km to the northeast of the WGC, and therefore should not be included on a model output plot entitled “westernmost Grand Canyon”. Consideration of the complete swaths of results for simulation #4 (Fig. 3F, Karlstrom et al. 2014 supplement) and the AFT simulation of Kelley et al. (2001) (Fig. 3D) reveals that some results are compatible with those of simulations #1-3 in permitting cold ($<30^{\circ}\text{C}$) temperatures by 65 Ma. Karlstrom et al. (2014)’s depiction of only a single path in Figure 3E (red curves) for these model results could be taken to imply that the data require the single tT path shown, which would lead to the incorrect conclusion that the data require temperatures warmer than 30°C long after 70 Ma, when they do not (see section 4.1). Finally, one of these simulations fit a sample with He dates that are analytically suspect and should not be used for tT interpretation (sim #6, see Section 5.1, light blue curve in Fig. 3E).

Ultimately, after considering these factors, only one simulation result (sim #5 in Fig. 3E) is inconsistent with early cooling to cold temperatures like that required by simulations #1-3 of Flowers and Farley (2012, 2013). This model’s requirement for elevated temperatures until the end of the Miocene stems from the mean FTL of $12.1\ \mu\text{m}$, but many relevant details are unavailable, including the measurement and calibration procedures.

5.4. Summary: Implications for when the WGC was carved

The Grand Canyon example shows how complex and confusing it can be to understand the origin of geologic interpretations when the data necessary for modeling are not published, and when model outputs are incompletely represented. From initial inspection of the contributions by Flowers and Farley (2012) and Karlstrom et al. (2014) it appears that their WGC thermochronologic datasets require dramatically divergent conclusions about this canyon segment's age (~70 Ma vs. <6 Ma). However, closer evaluation indicates that when one includes only samples actually from the WGC, if the full model outputs are considered, and if simulations using questionable data are rejected, all but one model result displayed by Karlstrom et al. (2014) in Figure 3E are compatible with those of Flowers and Farley (2012, 2013) (sims #1-3, Fig. 3A-C) and thus also are consistent with the ancient canyon interpretation. Additional work is needed to determine if the discrepant model result yielded by simulation #5 is sample specific, such as due to a localized reheating event by WGC Quaternary volcanism, or if it reflects a broader intercalibration issue with the AHe and AFT systems, suggesting that some aspect of the mutually agreed upon He diffusion kinetic (Fox and Shuster, 2014) or FT annealing models currently used by the thermochronology communities must be modified or augmented to reconcile the WGC datasets.

6. Concluding Remarks

Complete publication of all data necessary for thermal history modeling, together with clear documentation of model inputs and outputs, is necessary to enhance understanding of thermochronologic datasets and refinement of the methods being

533 applied. The proposed model input reporting table provides a mechanism to assist the
534 rapidly growing thermochronologic user base in key considerations of inverse tT
535 modeling. In particular, it provides an organizational framework that helps ensure that all
536 relevant information is reported, rather than relying on a loose collection of tables and
537 prose, and that the modeler will give each aspect of model input the care and attention a
538 scientific product requires. Additionally, for complex datasets in which divergent
539 conclusions are reached by different studies, transparency in the choice of model inputs
540 and outcomes would facilitate evaluation of how various assumptions influence the
541 interpretations, identify where discrepancies between datasets truly do or do not exist,
542 and thus aid in determining the extent to which intra- and inter-method calibration efforts
543 are needed. The Grand Canyon example shows how the origin of thermochronologic
544 interpretations can be clarified using this approach.

545 We hope that the suggested reporting table template will stimulate additional
546 community discussion about modeling philosophies and reporting formats. In the near-
547 term, including the reporting tables and HeFTy or QTQt model files in on-line
548 supplements would assist with attainment of the goals outlined here. Over the longer-
549 term, we envision that if clear, rigorous, and community-agreed upon definitions of Level
550 1 elements (i.e., for as many constituents of the model input file as practical) were
551 established, then a community database of model input files could add value in much the
552 same way as does a database of sample dates. If one or more modeling tools were capable
553 of ingesting such files and generating the swath of acceptable tT paths, this would readily
554 allow a user to reproduce a published Level 2 product. Moreover, if the Level 2 product
555 had an agreed upon format that includes the tT swath and all ancillary data used in its

generation (i.e., an output version of the model input file that is tagged to the swath), then a user could simply locate the Level 2 product from a publication (archived electronically), and either work directly with the reported swath of tT paths (i.e., move on to Level 3), or explore how the selection of Level 1 elements influences the Level 2 product. Such a database of model input and output files to archive and clarify the path of argument used to reach published interpretations would promote the transparency, value, and understanding of thermochronologic data in future investigations.

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References Cited

- Ault, A.K., Flowers, R.M., 2012. Is apatite U–Th zonation information necessary for accurate interpretation of apatite (U–Th)/He thermochronometry data? *Geochim. Cosmochim. Acta* 79, 60–78. doi:10.1016/j.gca.2011.11.037
- Brown, R.W., Beucher, R., Roper, S., Persano, C., Stuart, F., Fitzgerald, P., 2013. Natural age dispersion arising from the analysis of broken crystals. Part I: Theoretical basis and implications for the apatite (U–Th)/He thermochronometer. *Geochim. Cosmochim. Acta* 122, 478–497. doi:10.1016/j.gca.2013.05.041
- Burtner, R.L., Nigrini, A., Donelick, R.A., 1994. Thermochronology of lower Cretaceous source rocks in the Idaho-Wyoming thrust belt. *Am. Assoc. Pet. Geol. Bull.* 78, 1613–1638.
- Carlson, W.D., Donelick, R.A., Ketcham, R.A., 1999. Variability of apatite fission-track annealing kinetics :I. Experimental results 84, 1213–1223.
- Crowley, K.D., Cameron, M., Schaefer, R.L., 1991. Experimental studies of annealing of etched fission tracks in fluorapatite. *Geochim. Cosmochim. Acta* 55, 1449–1465.
- Dodson, M.H., 1973. Closure temperatures in cooling geological and petrological systems. *Contrib. to Mineral. Petrol.* 40, 259–274.

584 Donelick, R.A., Miller, D.S., 1991. Enhanced TINT fission track densities in low
585 spontaneous track density apatites using ^{252}Cf -derived fission fragment tracks: A
586 model and experimental observations. *Nucl. Tracks Radiat. Meas.* 18, 301–307.

587 Donelick, R.A., O’Sullivan, P.B., Ketcham, R.A., 2005. Apatite fission-track analysis.
588 *Rev. Mineral. Geochemistry* 58, 49–94.

589 Enkelmann, E., Jonckheere, R., Wauschkuhn, B., 2005. Independent fission-track ages
590 (ϕ -ages) of proposed and accepted apatite age standards and a comparison of ϕ -, Z-,
591 ζ -, and ζ_0 - ages: Implications for method calibration. *Chem. Geol.* 222, 232–248.

592 Farley, K.A., 2000. Helium diffusion from apatite: General behavior as illustrated by
593 Durango fluorapatite. *J. Geophys. Res.* 105, 2903–2914.

594 Farley, K.A., Shuster, D.L., Ketcham, R.A., 2011. U and Th zonation in apatite observed
595 by laser ablation ICPMS, and implications for the (U–Th)/He system. *Geochim.*
596 *Cosmochim. Acta* 75, 4515–4530. doi:10.1016/j.gca.2011.05.020

597 Farley, K.A., Shuster, D.L., Watson, E.B., Wanser, K.H., Balco, G., 2010. Numerical
598 investigations of apatite $4\text{He}/3\text{He}$ thermochronometry. *Geochemistry, Geophys.*
599 *Geosystems* 11, 1–18. doi:10.1029/2010GC003243

600 Farley, K.A., Wolf, R.A., Silver, L.T., Wolf, L.T., 1996. The effects of long alpha-
601 stopping distances on (U–Th)/He ages. *Geochim. Cosmochim. Acta* 60, 4223–4229.

602 Flowers, R.M., Farley, K.A., 2012. Apatite $4\text{He}/3\text{He}$ and (U–Th)/He evidence for an
603 ancient Grand Canyon. *Science* 338, 1616–9. doi:10.1126/science.1229390

604 Flowers, R.M., Farley, K.A., 2013. Response to Comments on “Apatite $4\text{He}/3\text{He}$ and (U–
605 Th)/He Evidence for an Ancient Grand Canyon.” *Science* (80-.). 340, 143–143.
606 doi:10.1126/science.1234203

607 Flowers, R.M., Kelley, S.A., 2011. Interpreting data dispersion and “inverted” dates in
608 apatite (U–Th)/He and fission-track datasets: An example from the US
609 midcontinent. *Geochim. Cosmochim. Acta* 75, 5169–5186.
610 doi:10.1016/j.gca.2011.06.016

611 Flowers, R.M., Ketcham, R.A., Shuster, D.L., Farley, K.A., 2009. Apatite (U–Th)/He
612 thermochronometry using a radiation damage accumulation and annealing model.
613 *Geochim. Cosmochim. Acta* 73, 2347–2365. doi:10.1016/j.gca.2009.01.015

614 Flowers, R.M., Shuster, D.L., Wernicke, B.P., Farley, K.A., 2007. Radiation damage
615 control on apatite (U–Th)/He dates from the Grand Canyon region, Colorado
616 Plateau. *Geology* 35, 447–450. doi:10.1130/G23471A.1

617 Flowers, R.M., Wernicke, B.P., Farley, K.A., 2008. Unroofing, incision and uplift history
618 of the southwestern Colorado Plateau from (U-Th)/He apatite thermochronometry.
619 Geol. Soc. Am. Bull. 120, 571–587. doi:10.1130/B26231.1

620 Fox, M., Shuster, D.L., 2014. The influence of burial heating on the (U–Th)/He system in
621 apatite: Grand Canyon case study. Earth Planet. Sci. Lett. 397, 174–183.
622 doi:10.1016/j.epsl.2014.04.041

623 Gallagher, K., 1995. Evolving temperature histories from apatite fission-track data. Earth
624 Planet. Sci. Lett. 136, 421–435. doi:10.1016/0012-821X(95)00197-K

625 Gallagher, K., 2012. Transdimensional inverse thermal history modeling for quantitative
626 thermochronology. J. Geophys. Res. 117, B02408. doi:10.1029/2011JB008825

627 Gautheron, C., Tassan-Got, L., Barbarand, J., Pagel, M., 2009. Effect of alpha-damage
628 annealing on apatite (U-Th)/He thermochronology. Chem. Geol. 266, 157–170.

629 Gleadow, A.J.W., Duddy, I.R., 1981. A natural long-term annealing experiment for
630 apatite. Nucl. Tracks Radiat. Meas. 5, 169–174.

631 Green, P.F., Duddy, I.R., Gleadow, A.J.W., Tingate, P.R., Laslett, G.M., 1986. Thermal
632 annealing of fission tracks in apatite 1. A qualitative description. Chem. Geol. 59,
633 237–253.

634 Gurnis, M., Flesch, L., Okaya, D., Peters, S., Walker, D., Ahern, T., Bolder, F.,
635 Arrowsmith, J.R., 2012. A preliminary strategic plan for EarthScope
636 cyberinfrastructure. White Pap.

637 Hourigan, J.K., Reiners, P.W., Brandon, M.T., 2005. U-Th zonation-dependent alpha-
638 ejection in (U-Th)/He chronometry. Geochim. Cosmochim. Acta 69, 3349–3365.

639 Johnstone, S., Hourigan, J., Gallagher, C., 2013. LA-ICP-MS depth profile analysis of
640 apatite: Protocol and implications for (U–Th)/He thermochronometry. Geochim.
641 Cosmochim. Acta 109, 143–161. doi:10.1016/j.gca.2013.01.004

642 Jonckheere, R., Enkelmann, E., Min, M., Trautmann, C., Ratschbacher, L., 2007.
643 Confined fission tracks in ion-irradiated and step-etched prismatic sections of
644 Durango apatite. Chem. Geol. 242, 202–217.

645 Karlstrom, K.E., Crow, R., Crossey, L.J., Coblenz, D., Van Wijk, J.W., 2008. Model for
646 tectonically driven incision of the younger than 6 Ma Grand Canyon. Geology 36,
647 835. doi:10.1130/G25032A.1

648 Karlstrom, K.E., Lee, J.P., Kelley, S.A., Crow, R.S., Crossey, L.J., Young, R.A., Lazear,
649 G., Beard, L.S., Ricketts, J.W., Fox, M., Shuster, D.L., 2014. Formation of the

650 Grand Canyon 5 to 6 million years ago through integration of older palaeocanyons.
651 doi:10.1038/NGEO2065

652 Kelley, S.A., Chapin, C.E., Karlstrom, K.E., 2001. Laramide cooling histories of Grand
653 Canyon, Arizona and the Front Range, Colorado, determined from apatite fission-
654 track thermochronology, in: Young, R.A., Spamer, E.E. (Eds.), Colorado River
655 Origin and Evolution. Grand Canyon Association, pp. 37–46.

656 Ketcham, R. a., Carter, A., Donelick, R. a., Barbarand, J., Hurford, A.J., 2007. Improved
657 measurement of fission-track annealing in apatite using c-axis projection. *Am.*
658 *Mineral.* 92, 789–798. doi:10.2138/am.2007.2280

659 Ketcham, R.A., 2005. Forward and inverse modeling of low temperature
660 thermochronometry data, in: Reiners, P.W., Ehlers, T.A. (Eds.), *Thermochronology.*
661 *Reviews in Mineralogy and Geochemistry*, pp. 275–314.

662 Ketcham, R.A., Carter, A., Hurford, A.J., 2015. Inter-laboratory comparison of fission
663 track confined length and etch figure measurements in apatite 100, 1452–1468.

664 Ketcham, R.A., Carter, A.C., Donelick, R.A., Barbarand, J., Hurford, A.J., 2007.
665 Improved modeling of fission-track annealing in apatite. *Am. Mineral.* 92, 799–810.

666 Ketcham, R.A., Donelick, R.A., Carlson, W.D., 1999. Variability of apatite fission-track
667 annealing kinetics : III . Extrapolation to geological time scales 84, 1235–1255.

668 Ketcham, R.A., Gautheron, C., Tassan-Got, L., 2011. Accounting for long alpha-particle
669 stopping distances in (U-Th-Sm)/He geochronology: Refinement of the baseline
670 case. *Geochim. Cosmochim. Acta* 75, 7779–7791. doi:10.1016/j.gca.2011.10.011

671 Laslett, G.M., Green, P.F., Duddy, I.R., Gleadow, A.J.W., 1987. Thermal annealing of
672 fission tracks in apatite 2. A quantitative analysis. *Chem. Geol.* 65, 1–13.

673 Lee, J.P., Stockli, D.F., Kelley, S.A., Pederson, J.L., Karlstrom, K.E., Ehlers, T.A., 2013.
674 New thermochronometric constraints on the Tertiary landscape evolution of the
675 central and eastern Grand Canyon, Arizona 216–228. doi:10.1130/GES00842.1

676 Murray, K.E., Orme, D.A., Reiners, P.W., 2014. Effects of U–Th-rich grain boundary
677 phases on apatite helium ages. *Chem. Geol.* 390, 135–151.
678 doi:10.1016/j.chemgeo.2014.09.023

679 Reiners, P.W., Ehlers, T.A., 2005. Low-temperature thermochronology: Techniques,
680 interpretations, and applications. *Rev. Mineral. Geochemistry*.

681 Shuster, D.L., Farley, K.A., 2003. $4\text{He}/3\text{He}$ thermochronometry. *Earth Planet. Sci. Lett.*
682 217, 1–27.

- Shuster, D.L., Farley, K.A., 2005. $4\text{He}/3\text{He}$ thermochronometry: theory, practice and potential complications. *Rev. Mineral. Geochemistry Low-Temperature Thermochronology Tech. Interpret. Appl.* (ed. P. Reiners T. Ehlers) 58, 181–203.
- Shuster, D.L., Farley, K.A., 2009. The influence of artificial radiation damage and thermal annealing on helium diffusion kinetics in apatite. *Geochim. Cosmochim. Acta* 73, 183–196.
- Shuster, D.L., Flowers, R.M., Farley, K.A., 2006. The influence of natural radiation damage on helium diffusion kinetics in apatite. *Earth Planet. Sci. Lett.* 249, 148–161. doi:10.1016/j.epsl.2006.07.028
- Spiegel, C., Kohn, B., Belton, D., Berner, Z., Gleadow, A., 2009. Apatite (U–Th–Sm)/He thermochronology of rapidly cooled samples: The effect of He implantation. *Earth Planet. Sci. Lett.* 285, 105–114. doi:10.1016/j.epsl.2009.05.045
- Vermeesch, P., Tian, Y., 2014. Thermal history modelling: HeFTy vs. QTQt. *Earth-Science Rev.* 139, 279–290. doi:10.1016/j.earscirev.2014.09.010
- Wernicke, B., 2011. The California River and its role in carving Grand Canyon. *Geol. Soc. Am. Bull.* 123, 1288–1316. doi:10.1130/B30274.1

Figure Captions

Figure 1. Interpretational framework showing the path from low level thermochronologic results and geologic observations to high level and potentially complex geologic interpretations.

Figure 2. (A) Shaded relief map for the Grand Canyon region with the Colorado River in blue. WGC segment marked by blue dots. Black square marks location of (B). (B) Shaded relief map for the WGC with sample locations. Mean AHe dates reported with 1σ standard deviation and number of analyses. AFT dates reported as central age and 1σ standard error. TL denotes samples with FTL data. Sample with AHe date in gray has overdispersed data. White rectangle marks WGC segment. River miles marked as RM.

(C) AHe date versus Grand Canyon river mile. Red symbols show the mean dates and 1σ uncertainties for the samples with 4-13% internal dispersion. The blue symbol marks the anomalous sample with excess random scatter (43% 1σ). Light gray circles denote the individual grain analyses for each sample. (D) Normalized $^4\text{He}/^3\text{He}$ step age plots for two apatites from CP06-69. (E) AFT date versus river mile, reported as the central age and 1σ standard error. (F) AFT mean track length versus river mile. Uncertainties are the reported 1σ standard error.

Figure 3. Outputs of the WGC models discussed in text. (A)-(C) Simulation #1-3 results for AHe and $^4\text{He}/^3\text{He}$ data depicted as individual tT paths, from Flowers and Farley (2012, 2013). (D) Simulation results for sample 98GC38 AFT data with the complete suite of output paths shown as fields, from Kelley et al. (2001). (E) Karlstrom et al. (2014) depiction of their simulation results, in which they show the simulation #3 results of Flowers and Farley (2013) in the background. The full suite of viable tT paths are not shown for 5 of their 6 simulations, nor are the tT constraints imposed on the models displayed. We annotated the figure to highlight key information necessary for evaluating the model results and the conclusions drawn from them. (F) Simulation #4 results for sample 01GC89 AHe and AFT dates, with the full swaths of statistically acceptable paths shown as fields. Green boxes on all plots are tT constraints imposed on the models (unknown for Fig. 3D). Simulation #1-3 results indicate cooling to $<30^\circ\text{C}$ by 70 Ma, so for reference the intersection of the gray dashed lines marks 30°C at 70 Ma on each model output plot.

Level 3:
Geologic interpretation

Level 2:
Thermal model outputs, which then can be horizontally integrated with other assumptions and geologic information

Level 1:
Thermal model inputs

Flowers et al.
Figure 1

Flowers et al.
Figure 2

Flowers et al.
Figure 3

Table 1. Thermal History Model Input Table

1. Thermochronologic data

(U-Th)/He data
 $^4\text{He}/^3\text{He}$ data
AFT data
Track length data

If data not presented in another table in paper, cite a specific data table in a reference

All data necessary for modeling must be reported (e.g. $^4\text{He}/^3\text{He}$ spectra steps, single grain AFT dates, individual track lengths)

Must include all necessary ancillary data that is used in the modeling (e.g., eU zonation, wt% Cl). When not available N/A should be reported and the default assumption in the model spelled out

Describe the uncertainties applied

If data from single or multiple samples are combined, explain how

2. Additional geologic information

Assumption (e.g., unconformity, max heating from independent burial depth estimate)

Explanation for the assumption

Source of information for this assumption

3. System- and model-specific parameters

He kinetic model (e.g., RDAAM)

FT annealing model: Model assumed, whether c-axis projection applied

Statistical fitting criteria: What constitutes a "good fit" what criterion is used for evaluating fit quality, what are the threshold levels, different methods may have different criteria and thresholds

Modeling code: specific code used and version #

Number of tT paths attempted

Table 2. Thermal History Model Input Table for Flowers and Farley (2012, 2013) simulations of Westernmost Grand Canyon thermochronology data

1. Thermochronologic data

Samples and data used in simulations

	Simulation #			Data Source ^a
	sim #1	sim #2	sim #3	
<u>AHe data</u>				
CP06-65, mile 225	x			(1)
CP06-69, mile 239	x	x	x	(1)
CP06-71a, mile 241	x			(1)
GC863, mile 248	x			(2)
<u>⁴He/³He Constraints^b</u>				
CP06-69 (c)	x	x	x	(3)
CP06-69 (d)	x	x	x	(3)
CP06-69 (b)			x	(3)

AFT dates and track-lengths: 98GC38 Only available AFT data for WGC. Used as geologic constraint in the simulations - see section 2 below. Could not be modeled because necessary data not reported.

Data treatment: Dates, uncertainties, and other relevant constraints

AHe data

Treatment: Each of the 4 samples was used as a separate constraint in HeFTy

He dates (Ma): Mean uncorrected He date of each sample. Uncorrected date corrected for a-ejection in HeFTy using Farley et al. (1996).

Error (Ma) applied in modeling: The 1 sigma sample standard deviation of each sample was applied if $\geq 12\%$. If $< 12\%$, then the 2 sigma sample standard deviation was applied.

r (um): Mean equivalent spherical radius of each sample

eU (ppm): Mean eU of each sample

eU zonation: representative profile for the simulations using each sample, data source (4)

CP06-65: profile D

CP06-69: profile D

CP06-71a: profile B

GC863: none, zonation too variable to select a representative profile

⁴He/³He Constraints^a

r (um): 69 um, the mean equivalent spherical radius of apatite analyzed from CP06-69

eU (ppm): 12 ppm, mean eU for the apatites analyzed by AHe for this sample

eU zonation: profile D for CP06-69

2. Additional geologic information

Assumption	Explanation and data source
At surface temperature of 20-25 °C by 0 Ma	25 °C based on modern shallow borehole data (Wernicke, 2011, Figure 11). 20 °C is probable endmember minimum estimate.
Peak temperature occurred at 100-80 Ma	Assumes peak temperature was attained near the timing of maximum burial. Cretaceous units preserved regionally in northern Arizona indicate that deposition continued until ~85 Ma (Nations, 1989; Flowers et al., 2008), consistent with peak burial attainment by that time. Increase to a broader, more conservative age range.
Simulations begin at peak temperatures of 120-110 °C	Available AFT data for the Grand Canyon, including the westernmost Grand Canyon, indicated complete apatite annealing at peak temperatures of > 110 °C (Dumitru et al., 1994; Kelley et al., 2001).

3. System- and model-specific parameters

He kinetic model: RDAAM for both AHe and ⁴He/³He simulations

Statistical fitting criteria: GOF values > 0.3 for AHe; GOF values > 0.32 for ⁴He/³He

Modeling Code: AHe uses HeFTy v1.8; ⁴He/³He uses Caltech code (unpublished)

Number of tT paths attempted: 8000 for all

^aData Source:

(1) - Flowers et al. (2008), Table DR1

(2) - Flowers and Farley, 2012, Table S6

(3) - Flowers and Farley (2012), Table S2

(4) - Flowers and Farley, (2012), Table S4

^b(b),(c),(d) are individual spectra for separate crystals from the sample

Table 3. Thermal History Model Input Table for Karlstrom et al. (2014) simulations of Westernmost Grand Canyon Thermochronology Data

1. Thermochronologic data

Samples and data used in simulations

	Simulation #			Data	All data needed	
	sim #4	sim #5	sim #6	Source ^a	for modeling published?	
<u>AHe data</u>						
01GC86, mile 243			x	(1)	no	Only eU and FT published;
01GC87, mile 252		x		(1)	no	insufficient information to back-
01GC89, mile 260	x			(1)	no	calculate grain size
<u>AFT dates</u>						
01GC86, mile 243			x	(2)	no	
01GC87, mile 252		x		(2)	no	Individual grain AFT dates necessary
01GC89, mile 260	x			(2)	no	for modeling are unpublished
<u>AFT lengths</u>						
01GC86, mile 243			x	(2)	no	Individual track-lengths necessary for
01GC87, mile 252		x		(2)	no	modeling are unpublished

Data treatment: Dates, uncertainties, and other relevant constraints

AHe data

Treatment: Each apatite analysis modeled independently but simultaneously for each sample, except for sample 01GC86, in which data for three grains is averaged.

He dates (Ma): Indicates that the "group average" is used, but also states each apatite analysis modeled individually. Uncorrected date corrected for α -ejection in HeFTy using Farley et al. (1996). Choice of grains modeled for 01GC87 is not indicated.

Error (Ma) applied in modeling: Unclear. Indicates that the error is the standard deviation of the age group, but one or two sigma not indicated.

r (um): Equivalent spherical radius of each grain or grains

eU (ppm): The eU of each analysis, or average

AFT data

Cl wt %: 0.1%

Initial mean track length: 16.17 um

Track length reduction standard: 0.893

2. Additional geologic information

Assumption	Explanation and data source
Peak temperature occurred in Cretaceous at ≤ 110 °C for most samples	Rationale not provided. When in Cretaceous not indicated.
Paleozoic near-linear increase toward max temperature	Represents Paleozoic deposition of sedimentary rocks
Simulations begin at 500 Ma	Represents near surface exhumation of basement samples before deposition of Cambrian Tapeats Sandstone.

3. System- and model-specific parameters

He Kinetic model: RDAAM

FT annealing model: Not indicated

FT c-axis projection: Not indicated

Modeling Code: HeFTy v1.7.4

Statistical fitting criteria: Default HeFTy values. GOF values >0.05 are acceptable fits. GOF values >0.5 are good fits.

Number of tT paths attempted: Following an initial simulation with $>100,000$ paths, additional tT constraints are imposed, and another simulation carried out. Variable attempted paths in the second model.

^aData Source:

(1) - Lee et al. (2013), Supplemental File 1

(2) - Lee et al., (2013), Table 2