



## Technical Note: A retroactive method for identifying subpopulations of zoned zircon in (U-Th)/He data

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**Abstract.** Zircon (U-Th)/He thermochronometry (ZHe) is a widely used tool for investigating and dating thermal events such as uplift, exhumation, incision, and plutonic emplacement, among others. The utility of this thermochronometer relies on its ability to measure and predict the production, distribution, and ultimately diffusion of radioactive decay products, a thermoregulated process. Natural zircon crystals frequently display internal chemical zonation as a result of precipitation environment, and metamorphism. This internal chemical heterogeneity unevenly partitions radioactive actinides, alpha particle production, and resultant accumulated radiation damage within the grain. The heterogeneous distribution of radiogenic He and radiation damage accumulation change the diffusion kinetics of these zircon, hindering our ability to calculate dates and ultimately develop thermal history interpretations. Models reveal that the effect of zoned actinides and associated radiation damage is magnified for samples characterized by negative ZHe date-eU trends produced by protracted thermal histories including extended residence in the partial retention zone. Measuring the degree and distribution of zoned radiation damage accumulation requires destructive characterization processes which precludes characterized zircon from whole grain ZHe dating. It is otherwise difficult to isolate zoned zircon during standard grain picking procedures, implying that many zircon grains that could be used for (U-Th)/He dating have spatially heterogeneous accumulated radiation damage. I developed a retroactive test to identify populations of potentially zoned zircon within a dataset utilizing the HeFTy v2.3.1 (Ketcham, 2025) forward modeler and “zoned” grain function. This test allows us to reproduce the behavior of endmember zonation styles in date-eU space, with the ultimate goal of identifying and reclaiming these data to develop more robust thermal history interpretations. Considering zircon damage zonation may be helpful when interrogating samples with complex ZHe date-eU patterns that are otherwise difficult to interpret.

### 1 Introduction

Zircon (U-Th)/He thermochronology (hereafter ZHe) leverages accumulated radiation damage within grains for calculating damage-diffusivity ratios and ultimately grain dates, informing our thermal history interpretations. For a given sample, the zircon population is inherently diverse in effective Uranium concentration ( $eU=[U]+.238[Th]$ ; Cooperdock et al., 2019). Most natural zircon present with chemically heterogeneous internal zones with variable eU concentrations (Corfu et al., 2003). Higher eU concentrations result in



40 increased production of alpha particles, and an increased rate of alpha ejection recoil and  
resultant radiation damage (Shuster and Farley, 2009). Internal zonation of eU in  
combination with a samples thermal history can impact intra-grain distribution of  
accumulated radiation damage, concentrating damage in areas enriched in eU. This  
implies that zonation in zircon influence date-eU patterns and therefore our thermal  
history interpretations (Anderson et al., 2020b).

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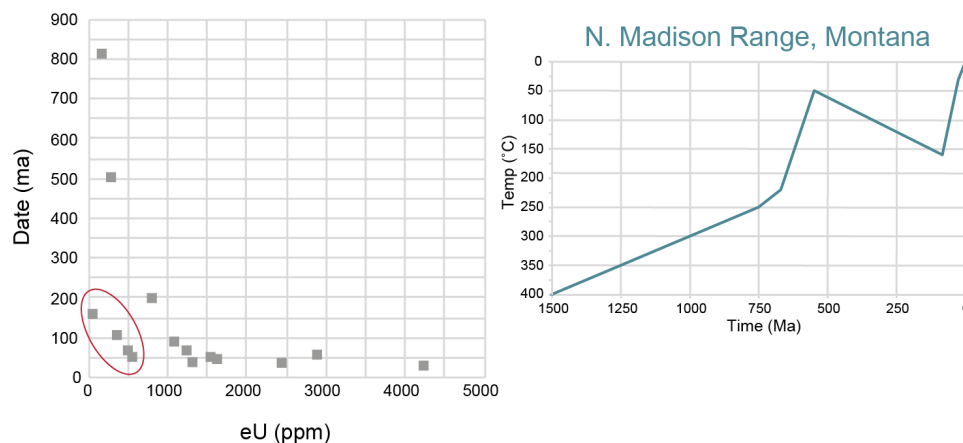
Zircon crystals with internal chemical heterogeneities are commonplace and are caused  
by variable magmatic composition during crystallization, resorption, xenocrystic cores,  
and metamorphic overgrowth, among other processes (for a detailed discussion of zircon  
morphology, see Corfu et al., 2003). Commonly, chemical heterogeneities in zircon  
50 present as narrow, concentric growth bands which record oscillating trace element  
content in the parent melt (e.g. Hoskin, 2000; Fowler et al., 2001). Less frequently, the  
processes of resorption and metamorphic overgrowth result in strong core-rim textures  
(e.g. Hanchar and Rudnick, 1995, Corfu et al., 2003). These core-rim textures in zircon  
are still common enough for routine utilization in in-situ laser ablation U-Pb analysis of  
55 igneous and metamorphic rocks from complex systems (i.e. Bowring et al., 1989).

Despite the prevalence of these core-rim textures in magmatic and metamorphic zircon,  
heavily zoned zircon are often overlooked in ZHe studies either due to difficulty identifying  
or characterizing zoned grains, or due to the complex alpha ejection correction required  
60 to analyze these grains. Previous studies have addressed the utility of picking zircon  
based on visual metamictization (a proxy for radiation damage accumulation; Ault et al.,  
2018; Armstrong et al., 2022), however it is difficult to determine internal characteristics  
like zonation using standard grain picking procedures for ZHe. Characterization of internal  
zonation requires zircon grains to be mounted in epoxy and polished to the grain's half-  
65 width, a destructive process that precludes these grains from whole-grain ZHe analysis  
(Lenz et al., 2020). Characterization of grains prior to ZHe analysis is not always feasible  
due to analytical expense, low zircon yields, and time constraints. Without detailed  
characterization of zoned zircon from within a sample, or the ability to differentiate zoned



grains with plain light microscopy, core-rim zoned grains may inadvertently be selected  
70 for whole grain ZHe analysis.

The range of radiation damage produced by variable intra-sample zonation styles affects  
the (U-Th)/He date by retaining or losing He at different rates than those grains without  
significant or zoned radiation damage (Farley et al., 2011). He diffusivity rates in zircon  
75 are affected by accumulated radiation damage within the crystal lattice: non-uniform  
radiation damage accumulation yields non-uniform He production and diffusivity, resulting  
in inaccurate alpha-ejection corrections ( $F_T$ ; Farley et al., 1996; Hourigan et al., 2005;  
Farley et al., 2011; Guenther et al., 2013). This non-uniform He diffusion behavior, in  
combination with accumulated radiation damage, result in the over- or underprediction of  
80 grain date when calculated using standard  $F_T$  corrections (Farley et al., 2011; Guenther  
et al., 2013; Anderson et al., 2020b). This date dispersion manifests as complex or  
scattered patterns in date-eU space, often causing (U-Th)/He date disparities over small  
eU ranges (<50 ppm difference in eU). This disparity between sample dates over small  
eU ranges is most apparent in samples with complex thermal histories, or prolonged  
85 residence in the partial retention zone (Fig. 1). Significant date scatter or outlier data may  
be caused by core-rim zoned zircon. Once identified, these outliers caused by core-rim  
zonation can be 1) removed from the study on the basis of texture or chemistry, or 2)  
treated as an additional thermochronometer with different kinetics (i.e. closure  
temperature, alpha ejection corrections) and sensitivities in time-temperature space than  
90 standard ZHe data.



**Figure 1: Zircon (U-Th)/He data from the northern Madison Range, Montana (Kaempfer et al., 2021). Data are negatively correlated in date-eU space, with outliers at low eU (circled in red). The second panel shows the published forward modeled derived time-temperature path for this dataset. This time-temperature path is ultimately used for predicting hypothetical grain ages in Fig. 3.**

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The aim is to identify subpopulations of zircon within a dataset whose ZHe dates are affected by internal zonation of radiation damage, either to remove these grains from consideration or to expand the scope of our interpretations. Forward modeling can be used as a tool for visualizing subpopulations of zoned grains within a dataset by replicating the He diffusion behavior of heavily zoned and radiation damaged grains in date-eU space. These grains, once identified, can be leveraged for a more robust thermal history interpretation. The replication of grain behavior is produced through the use of hypothetical core-rim zoned zircon with eU concentrations and Rs values representative of a dataset. Herein I present a dataset of core-rim zoned hypothetical grains across the spectrum of eU; this dataset can be forward modeled using the time-Temperature path of your existing data to reproduce the behavior of zoned grains in date-eU space. This methodology is demonstrated using data from the northern Madison Range, Montana, consisting of Precambrian zircon with notable date dispersion at low eU (Kaempfer et al., 2021).

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## 2 Methodology



This methodology covers the parameters and design of the hypothetical grain dataset, and its intended uses. Section 2.1 covers the development of the hypothetical dataset, including grain size and zone width, and calculating zone eU concentrations. Section 2.2 details the workflow of predicting grain dates using hypothetical grains, as well as adjusting parameters of the hypothetical zoned grains. Section 2.2 also discusses the comparison of hypothetical grains to real data in date-eU space.

## 2.1 Hypothetical zoned zircon parameters

Hypothetical zoned zircon grains were designed with several factors in mind: 1) zonation style must be generally representative of core-rim zonation textures, 2) grain  $R_s$  (spherical radius, used in calculating  $F_T$ ) must be generally representative of natural zircon, 3) eU concentrations must capture the range of observed eU concentrations in a given dataset. To this end, the hypothetical grains presented herein are generalized in terms of grain size and zone width in order to highlight the effect of zoned eU concentration, radiation damage, and He diffusion. Importantly, I utilize zone widths greater  $20\mu\text{m}$  to represent those grains whose zones are wider than the alpha-ejection stopping distance (Hourigan et al., 2005).

The presented set of hypothetical grains have a uniform  $R_s$  of  $60\mu\text{m}$ , and internal zones have a set width of  $30\mu\text{m}$  (half of the  $60\mu\text{m}$   $R_s$ ) in order to best represent natural zircon with core-rim textures. Concentration profiles of these hypothetical grains exhibit a) maximum eU concentration in the rim and b) maximum eU concentration in the core. Bulk eU values used in hypothetical testing are chosen so that they represent the full range of eU in a given sample. It should be noted that I assume U is the only contributor to eU, as the intricacies of variable U, Th, and Sm contributions to eU is beyond the scope of this study. Additionally, I assume a minimum eU concentration of 50 ppm for non-enriched zones. Bulk U concentration is increased in the enriched zone in order to maintain the correct bulk eU value for the grain. Equations (1) and (2) calculate the necessary U concentration in the core or rim zone necessary to maintain correct bulk eU concentrations in grains with core and rim zones equal to half the  $R_s$ , and a



minimum eU of 50 ppm. The concentration of U in enriched core or rim zones changes linearly according to the following functions:

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$$Core [U] = 7.96 * [desired\ eU] - 347.72 \quad (1)$$

$$Rim [U] = 1.14 * [desired\ eU] - 7.18 \quad (2)$$

Grain parameters, eU concentrations by zone, and zone width are presented in Table 1.

150 **Table 1. Parameters for hypothetical zoned zircon, including the necessary [U] to maintain the correct bulk eU. Files corresponding to each hypothetical grain are provided in the appendix.**

Table 1. Hypothetical zoned zircon parameters

Zone style	Bulk eU (ppm)	Rs (µm)	Core [U]	Core radial depth (µm)	Rim [U]	Rim radial depth (µm)	HeFTy file name
Enriched Core	100	60	448.0	0-29.9	50	30-60	Core100.txt
	250	60	1641.5	0-29.9	50	30-60	Core250.txt
	500	60	3630.8	0-29.9	50	30-60	Core500.txt
	1000	60	7609.3	0-29.9	50	30-60	Core1000.txt
	1500	60	11587.8	0-29.9	50	30-60	Core1500.txt
	2000	60	15566.3	0-29.9	50	30-60	Core2000.txt
	2500	60	19544.8	0-29.9	50	30-60	Core2500.txt
Enriched Rim	5000	60	39437.3	0-29.9	50	30-60	Core5000.txt
	100	60	50	0-29.9	107.2	30-60	Rim100.txt
	250	60	50	0-29.9	278.7	30-60	Rim250.txt
	500	60	50	0-29.9	564.7	30-60	Rim500.txt
	1000	60	50	0-29.9	1136.4	30-60	Rim1000.txt
	1500	60	50	0-29.9	1708.2	30-60	Rim1500.txt
	2000	60	50	0-29.9	2280.0	30-60	Rim2000.txt
	2500	60	50	0-29.9	2851.8	30-60	Rim2500.txt
5000	60	50	0-29.9	5710.8	30-60	Rim5000.txt	

155 **2.2 Predicting ages using the HeFTy forward modeler**

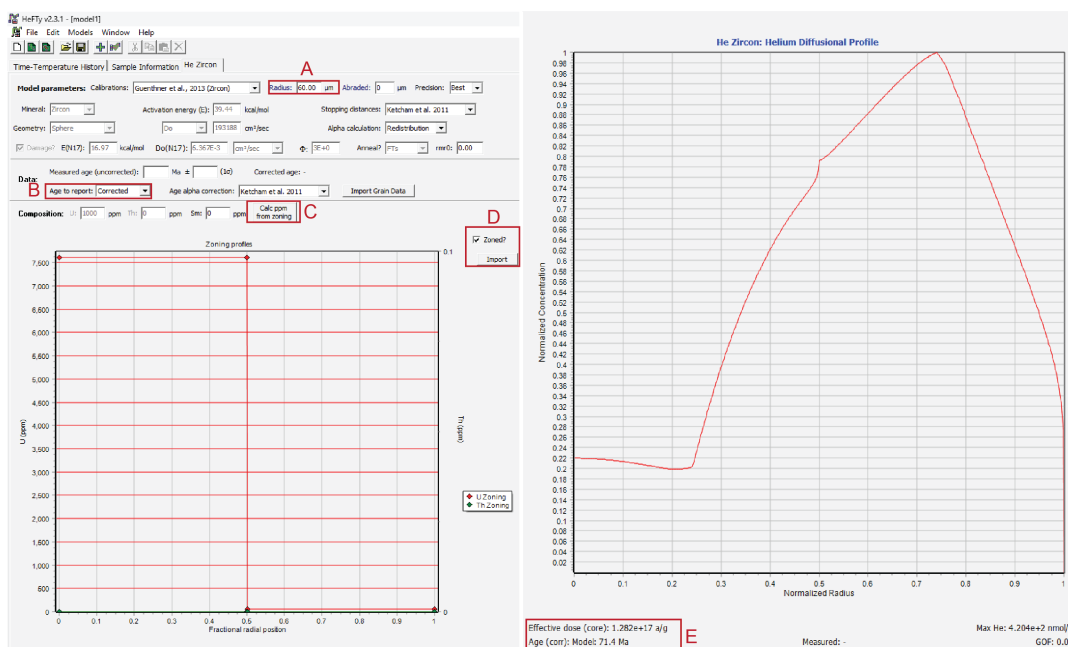
Predicted ages of hypothetical grains may be applied retroactively to identify outlier sample data. It is necessary, therefore, to use a best-fit time-temperature path that predicts inlier data to understand how core-rim zoned grains behave under those same conditions. Forward modeled date predictions for hypothetical zoned grains are calculated through HeFTy v2.3.1 using the ZRDAAM kinetic model (Ketcham, 2025; Guenther et al., 2013). HeFTy allows users to vary the forward model parameters, and

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to directly adjust the position and eU concentration of internal zones (Fig. 2, Fig. A1). For the hypothetical dataset presented here, I use the Guenther et al., 2013 kinetic model which accounts for accumulated radiation damage and annealing of grains (Fig. 3A). I utilize the Ketcham et al., 2011 calculations of alpha stopping distances for grains of different geometries, and redistribution of alpha particles (Fig. 2B).

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**Figure 2: He model input page and corresponding He diffusion profile with age prediction for a core-enriched hypothetical grain, both in HeFTy (Ketcham, 2025).**

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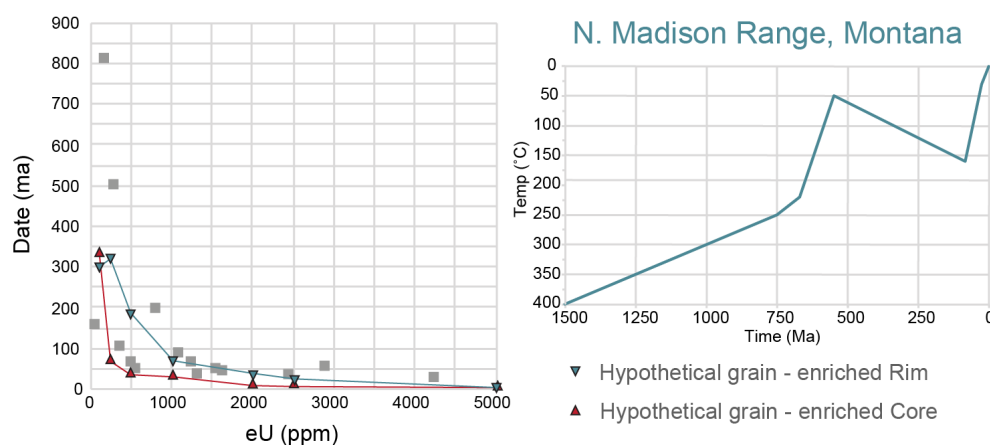
**Inset boxes indicate: A) grain radius input, B) reporting corrected or NCZ-corrected ages, C) optional confirmation of bulk eU using “Calc ppm from zoning”, D) zoned grain function and grain file import, and E) reported age and core effective dose report.**

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Herein I describe the intended workflow for using hypothetical zoned grains to retroactively identify zoned grains within a sample dataset. (Fig. A1). To use HeFTy to predict ages for hypothetical grains, use an appropriate time-temperature path for the sample data, and the He model settings described above. Using a time-temperature that best predicts inlier data is crucial, forward model age prediction relies on the base



180 assumption that all grains experience the same thermal history. Once settings are  
 adjusted, individually import the data file for each zonation style and bulk eU  
 concentration (Fig. 2D; Table 1, data files provided in supplement). Optionally, the bulk  
 eU concentration can be confirmed using the [Calc ppm from zoning] function (Fig. 2C).  
 HeFTy outputs predicted ages, reported as corrected or NCZ-corrected, and diffusion  
 185 profiles for each hypothetical grain He model input (Fig. 2E). Record the predicted ages  
 from relevant zonation styles and eU concentrations and plot these data against  
 corresponding sample data to compare the date-eU distribution (Fig. 3). This process  
 may be iterated, adjusting the Rs and the bulk eU of hypothetical grains using Eq. (1) and  
 (2) to best represent the sample data (Fig. 2A). There are four likely outcomes of this  
 190 comparison, described below (Fig. A1 outcomes A, B, C, and D).



**Figure 3: Comparison of hypothetical grains plotted against sample data from the northern Madison Range (Kaempfer et al., 2021). Ages for hypothetical grains were predicted using the HeFTy forward modeler, and the published time-temperature path for the northern Madison Range (second panel). Hypothetical grains with enriched rims, shown with blue triangles, exhibit a slight positive date-eU correlation before predicted dates correlate negatively with eU over 250 ppm. Hypothetical grains with enriched cores, shown with red triangles, record negative date-eU correlation at all eU concentrations. These hypothetical grains with enriched cores overlap with the outlier data at low eU (see Fig. 1)**

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First, hypothetical data that overlap with outlier data are likely to represent zoned grains within the sample (Fig. A1, outcome A). Figure 3 exhibits overlap between hypothetical core-enriched grains and an outlier population between 250-500 ppm eU. In this case, 205 the core-enriched zonation style, bulk eU, and hypothetical grain Rs are representative of core-rim zoned grains in the sample data. This implies that the outlier data at low date-low eU may be the result of zoned zircon with enriched cores suggesting core-enriched zoned zircon were inadvertently picked for (U-Th)/He analysis (Kaempfer et al., 2021).

210 The second outcome is hypothetical data that plots nearby outlier data, but does not directly overlap (Fig. A1 outcome B). In this case zonation is a likely explanation for sample data scatter, however the hypothetical grains do not fully represent zonation styles or Rs in the sample data. In this scenario I recommend adjusting the bulk eU concentrations of the hypothetical data using Eq. (1) and Eq. (2) and iterating the age 215 prediction and data comparison processes. Additionally, the Rs of the hypothetical zoned zircon may be adjusted through the HeFTy He Model input page (Fig 2). Adjusting the hypothetical zoned grains' Rs does not affect the eU concentration in enriched zones.

In the third outcome, hypothetical zoned grains do overlap with either inlier or outlier data 220 in date-eU space (Fig. A1 outcome C). The parameters of the hypothetical grains may not be representative of the zonation styles, zircon Rs, and eU concentrations of zircon from that sample. Alternatively, scatter in this sample may be unrelated to zonation. I recommend re-testing hypothetical grains with adjusted bulk eU concentrations and Rs, as in outcome B.

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Lastly, the distribution of hypothetical data overlaps with the inlier data (Fig. A1 outcome D). In this scenario, core-rim zoned grains are not the primary source of intrasample scatter. The hypothetical grains may not be representative of the zonation styles or eU concentrations of zircon from that sample. Alternatively, the hypothetical grains are not 230 sensitive to the sample's time-temperature path.



This workflow recommends iteratively retesting hypothetical grains depending on how they overlap with inlier and outlier sample data. Hypothetical grain  $R_s$  is adjusted simply through changing the grain's radius through the model parameters panel on HeFTy (Fig. 2). Zone widths are converted from depth to fractional radial widths when files are input into Hefty, therefore changing the grain radius through the HeFTy model parameters panel does not change the proportional width of zones. Bulk eU concentrations may similarly be adjusted to best represent eU distribution in sample data. Changing the bulk eU value requires recalculating the U concentration of enriched zones using Eq. (1) and (2) and editing the concentration values in the input files accordingly (i.e. core100.txt). These edited files are then remodeled using the method outlined above.

### 3 CONCLUSION

The intent of this study, and provided hypothetical dataset, is to identify core-rim zoned zircon within a sample dataset. These core-rim zoned zircon introduce date disparity in date-eU space, particularly for samples with complex or protracted thermal histories, due to their heterogeneous internal distribution of accumulated radiation damage and resultant He diffusion kinetics (Hourigan et al., 2005, Anderson et al., 2020b). This method shows the likely date-eU distribution of core-rim zoned zircon using hypothetical zoned grains forward modeled using a samples time-temperature path, allowing the user to identify probable subpopulations of zoned sample zircon. Plotting hypothetical data against sample data in date-eU space has four potential outcomes: outcome A) overlap between hypothetical zoned grains and outlier data suggesting indicating intrasample scatter may be caused core-rim zoned zircon; outcomes B and C) hypothetical zoned grains do not overlap with outlier data, suggesting bulk eU, zonation style and  $R_s$  of hypothetical data are not representative of outliers; outcome D) hypothetical data overlaps with inlier sample data indicating that core-rim zonation does not contribute to date-eU scatter.

This workflow identifies those grains within a sample *likely* to exhibit internal core-rim zonation; the style and severity of zonation within a sample should be characterized and confirmed independently. There are multiple ways to treat these outlier data following

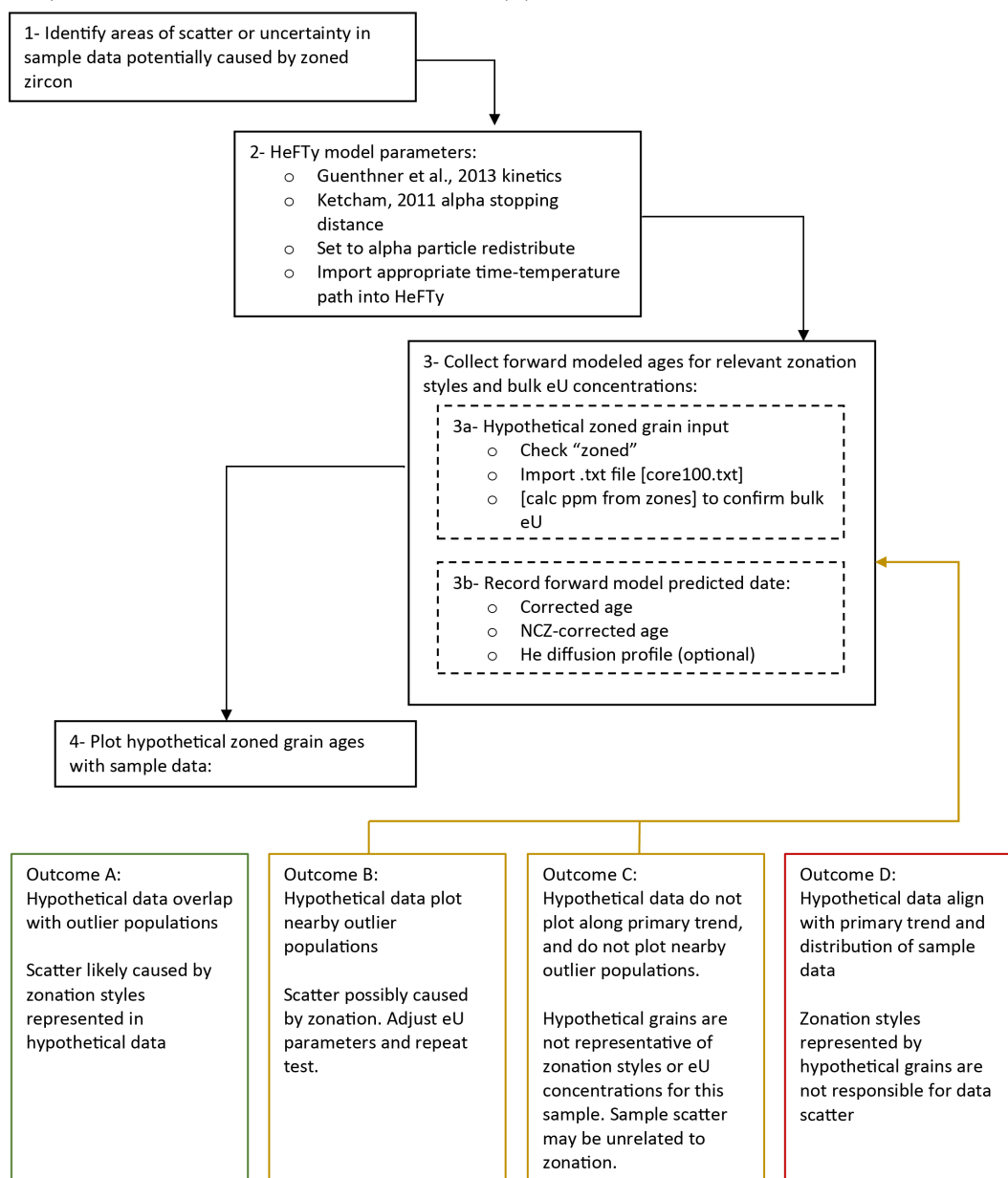


identification, depending on the scope and intent of the study. These sample grains  
identified as core-rim zoned may justifiably be removed from consideration on the basis  
265 of unpredictable kinetics among other reasons. Optionally, these potentially zoned grains  
may be reincorporated into the sample data as single-grain thermochronometers, as an  
alternative to binning and averaging date disperse grains at similar eU concentrations  
(Anderson et al., 2020b). Finally, these outlier data may be modeled independently of  
inlier data, treated as a separate thermochronometric system with specific kinetics,  
270 potentially yielding a more robust multi-system thermal history interpretation.

## **APPENDIX A**



HeFTy workflow for retroactive identification of zoned zircon subpopulations:



275 Fig. A1: Workflow in HeFTy



### Data Availability

Data presented in this work is available at zenodo.org via <https://doi.org/10.5281/zenodo.19864154> (Kaempfer, 2026).

### Supplement link

#### 280 Author contributions

All work and writing was completed by JMK.

### Competing interests

JMK claims no competing interests.

### Disclaimer

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#### 290 Review statement

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