A comment on Fox et al. gchron-2022-23: Is zircon (U–Th)/He kinetic model uncertainty [only] an issue for thermochronometric resolution of the Great Unconformity?

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The manuscript by Fox et al. highlights the impact of uncertainty on time-temperature (t–T) inversions with respect to the widely used (U–Th)/He kinetic model that describes radiation damage effects on ^{4}He diffusion in zircon (ZRDAAM; Guenthner et al., 2013). The focus on diffusion kinetic uncertainty is timely and commendable—hopefully stimulating further work to understand foundational aspects of zircon thermochronometry. A similar conclusion has been discussed for nearly a decade in the published literature regarding kinetic model calibration and uncertainty (e.g., Powell et al., 2016; Anderson et al., 2017; Johnson et al., 2017; Mackintosh et al., 2017; McDannell et al., 2019; Guenthner, 2021), but to date, few attempts have been made to formally account for uncertainties directly in the most commonly used thermal history modeling programs, nor have many more comprehensive laboratory diffusion experiments been undertaken to better understand how radiation damage affects diffusivity for a broader suite of natural zircons (e.g., Ginster et al., 2019). Kinetic uncertainties extend to the apatite (U–Th)/He system as well (e.g., Flowers et al., 2009; Gautheron et al., 2009; Fox and Shuster, 2014; Recanati et al., 2017; Willett et al., 2017; Guo et al., 2021). Thus, (U–Th)/He kinetic uncertainty has been a well-known problem that perhaps has not been addressed more decisively because the models have been considered good enough for most geologic applications.

1 Kinetic model uncertainty

Estimates of the effects of kinetic uncertainty for the (U–Th)/He system are rarely, if ever performed. Empirically derived results suggest α-damage kinetics can be explained to first order by general characteristics of fission-track annealing (Guenthner et al., 2013, Ketcham et al., 2013), but there are differences in detail and gaps in our understanding remain (Ginster et al., 2019; Guenthner, 2021). Thus the ZRDAAM kinetic model recalibration presented in the Fox et al. preprint is also by definition imperfect. So it becomes a question of what level of kinetic model uncertainty are we willing to live with and when does it cause significant t–T inversion inaccuracy? This is probably a challenge relevant to all timescales but it may be more important for certain geologic scenarios (e.g., Guenthner, 2021) and becomes especially difficult to quantify in deep time—since geological benchmarks are scarce and laboratory kinetic extrapolations become murky (Ketcham, 2019). Regardless of personal bias, seemingly casting "thermochronometric uncertainty" as only a concern for resolving the origin of the Great Unconformity is inappropriately narrow*.

2 Parameter correlations

The authors raise important points about parameter correlations and how different kinetics may change model results due to differences in damage annealing. Correlations between ZRDAAM diffusion kinetic parameters such as activation energy (E_a) and frequency factor (D_0) are important for assessing model accuracy and addressing uncertainties—yet extrapolations between theoretical minimally damaged and highly damaged amorphous zircons are still based on real, but limited, laboratory data. So while it is a useful exercise, it is nonetheless inhibited by the data grounding the established radiation damage relationship. Of course, E_a and D_0 are dependent on time-temperature conditions. Time and temperature are also correlated and any change in temperature at one time can be compensated

A detail worth noting is that Fox et al. stated (lines 91–92): "...the uncertainties in the radiation damage model make it challenging to accurately infer the timing and magnitude of unconformities in the deep past*". Thermochronological methods lack the temperature sensitivity to determine the final erosional event that results in an unconformity, and the erosional surface itself is inherently a feature terminated and preserved by sedimentation. McDannell et al. (2022a) were not 'dating the unconformity' but were instead placing limits on the timing, magnitude, and most importantly the spatial pattern of widespread rock cooling and exhumation that led to formation of the Great Unconformity in North America.

by an opposing temperature change at another time (e.g., Willett, 1997). Isolating kinetic uncertainty in models is important, however, ignoring other factors that may affect t–T inversions makes it hard to evaluate the absolute effects and practicality of such measures.

- Does reduction of the uncertainty of the diffusion data for the critically important damaged N17 zircon (lines 189–192) drive the 'excellent' MCMC recovery of E_a and D_0 (their fig. 2), and does this in any way have an effect on the poorer recovery (with respect to the canonical values) of the parameters for the undamaged crystal?
- Can the Fox et al. ZRDAAM E_a and D_0 calibration values simply be resampled using MCMC in a Bayesian t–T inversion, and if so, how would that affect thermal history recovery?

3 The effects of additional constraints on inversions results?

Fox et al. presented QTQt inversions (Gallagher, 2012) without imposed constraints (latter commonly represented as t–T boxes through which candidate histories must pass). To be clear, the so-called "unconstrained" models in McDannell et al. (2022a) were explicitly shown to assess the t–T sensitivity of the data during recursive modelling and comparison of alternate models with t–T boxes. Gallagher (2021) most recently discussed this QTQt modelling strategy in some detail. Other commentary has improperly dismissed that class of models as 'invalid' due to misunderstandings about their meaning and purpose (Flowers et al., 2022). However, such exercises prove useful and informative for validation of near-endmember models against the geologic record, rather than just simply forcing the data to conform to an uncertain, presupposed geologic model (see McDannell et al., 2022b). Any models presented in the former way should be viewed within the bounds of the kinetic assumptions (that are held fixed between inversions). Evaluating different inversion parameterizations with other geological constraints and/or associated uncertainties are valuable and motivationally transparent. Unconstrained inversions without many t–T boxes are undoubtedly affected by uncertainty and parameter correlations (as are those with boxes). Yet, systematic uncertainties may pose a more dubious problem for inversions that enforce *many* optimistically certain t–T constraint boxes based on interpretive assumptions.

- How do known physical geologic constraints affect the Fox et al. QTQt inversions? It is understood that examining kinetic parameter uncertainty in isolation was a goal of the paper, however, the effects of that uncertainty on the thermal histories would likely change with imposed constraints—this should be investigated and compared to the baseline case.
- Do geologic constraints imposed in a thermal history inversion impact the covariance/correlations between (kinetic) parameters?
- How do the observed vs. predicted zircon (U–Th)/He (ZHe) dates compare for the different QTQt inversions (i.e., Gallagher, 2016)?
- Does inverting multiple thermochronometers (as was done in the McDannell et al. 2022a MRVT models) reduce model non-uniqueness and change t–T resolution?

4 Posterior probabilities

It is unclear how much the Fox et al. thermal histories actually change in detail (their fig. 5), and if such changes quantitatively impact interpretations for parts of t–T space where the thermochronometer data are most sensitive. For example, their QTQt models mostly show differences in the pre-1000 Ma thermal history for the Minnesota River Valley Terranes (MRVT; McDannell et al., 2022a), which is not well constrained by data due to Neoproterozoic (and later) thermal resetting. However, by our account, the late Neoproterozoic cooling and episodic Phanerozoic reheating history is quite similar between the models implementing the original ZRDAAM kinetics and recalibrated high/low amorphous frequency factor kinetics. Fox et al. asserted that (line 251): "*Results show that while the general trend of the cooling is very similar, the posterior probabilities are all quite different (figure 5).*" The relative posterior probabilities seem comparable across all models except for the extremely linear regions of high probability (see below). The first-order differences in the recovered history styles, or at least the posterior probabilities of the accepted paths compared to the inversions in McDannell et al. (2022a) [that were run for much longer in QTQt], indicate that there may be procedural reasons for these discrepancies.

- Could the posterior probability change with increased MCMC sampling?

- Could the number of model iterations required for the posterior distribution to become stationary change depending on the kinetics?

4.1 MCMC burn-in and ZHe uncertainties

In all three of the Fox et al. QTQt models, the regions of t–T space with the highest relative probabilities are very "linear"—a possible cause for this could be that the burn-in for the inversions was too short (and/or restarted QTQt inversions began with a poor model). We discovered analogous posterior probability behavior related to burn-in in preliminary QTQt tests for the MRVT samples (McDannell et al. 2022a; published models $\geq$ 500,000 burn-in/post-burn-in iterations). We ran QTQt model tests with up to 1,500,000 burn-in iterations and 1,000,000 post burn-in iterations—the accepted paths typically gained structure with longer run times. Much longer burn-in periods are required for deep-time inversions spanning billions of years with large (multi-)thermochronometer datasets.

Another likely reason for the linearity in the regions of high relative posterior probability in the accepted t–T paths may be that, as far as we can tell, the Fox et al. QTQt models allowed the ZHe age uncertainties to be resampled up to 1–2× the input age error (K. Gallagher, pers. comm.). Fox et al. used the same the same Minnesota QTQt input ZHe data file was used in McDannell et al. (2022a). The problem with that approach is that the Minnesota dates in McDannell et al. (2022a) already underwent a form of Empirical Bayes error resampling prior to inverse modelling (see fig. S15 in that paper). The internal analytical uncertainties were used to calculate the 'external uncertainty' by creating a Gaussian kernel or normal probability density function in eU space centered on each uncorrected ZHe date (eU = effective uranium = U+0.238*Th). A 100-ppm eU kernel was taken to represent the range over which zircon grains with similar eU should have similar ages and the Empirical uncertainty was estimated by summing the internal and external uncertainties in quadrature (code available: `https://github.com/OpenThermochronology/EmpiricalBayes`).

Therefore, Fox et al. allowed the uncertainties on the input data to be much too large, which essentially causes a loss of apparent complexity in the observed date-eU pattern and allows the data to be easily reproduced—resulting in more simple t–T paths being accepted (regions of t–T space with high relative probability are linear). For example, the oldest 770 Ma zircon had an input Empirical Bayes uncertainty of ± 100 Myr but this was allowed to be sampled up to ± 200 Myr in the Fox et al. inversions. Due to this, we assume that the fits between the observed and predicted data are poor (i.e., many of the predictions are at the margin of acceptability), but that is unable to be evaluated in the preprint. A similar discussion in McDannell and Keller (2022) touched on the issue of uncertainty estimation for apatite (U–Th)/He data and how if uncertainties become too large then all t–T sensitivity is lost (see their Fig. S1). In QTQt this can result in simple linear histories being accepted more often. Such a model may be interpreted as geologically meaningful but that may not be appropriate (e.g., Gallagher, 2021). Simple t–T models are merely due to inadequate sensitivity/resolution, which could be sourced from the kinetics or the chronometer data. These outcomes are not just limited to Bayesian methods. Other software that utilize pure Monte Carlo search methods instead rely on many "exploration boxes" to delineate the model space, therefore, loss of sensitivity due to outsized data errors would probably never be recognized by the modeller. In many cases this would also be a welcome effect because it would allow more paths to be found more easily with a nondirected MC algorithm—this means that boxes (based on assumptions) could have more influence on the thermal history results than the (U–Th)/He data.

4.2 Timing of cooling

Fox et al. expressed (lines 96–98): "*Using QTQt, we show that different diffusion kinetics can lead to the onset of cooling for resolved thermal histories from inverse methods varying by hundreds of millions of years.*" and lines (253–254): "*In particular, the part of the thermal history that appears well resolved by the data changes from 1000 Ma to 1500 Ma depending on the choice of radiation damage parameters.*" These statements seem based on interpretation of where the initial timing of higher relative probability begins within the different QTQt models. Considering the potential limiting circumstances surrounding their date uncertainties being too large (and/or incomplete burn-in?) this seems a tenuous conclusion. Their interpretation overlooks the consistent Neoproterozoic cooling present in all of their models. In addition, there is no obvious reason why 'cooling onset' would necessarily correlate with high posterior probability. The time of peak cooling when the first derivative of a cooling curve is maximized is perhaps a better metric to consider (fig. 1). The apparent differences in resolution in their models is not necessarily because of the choice of radiation damage parameters. The fact that Neoproterozoic cooling is present in the Fox et al. models but low probability suggests that there are possible issues surrounding burn-in or overall poor t–T resolution due to overestimated ZHe uncertainties.

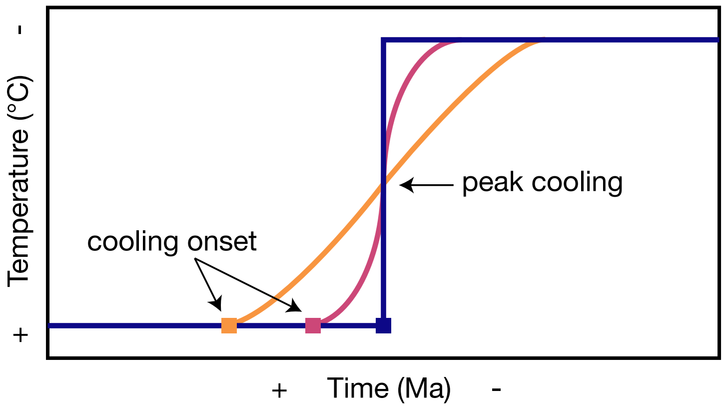
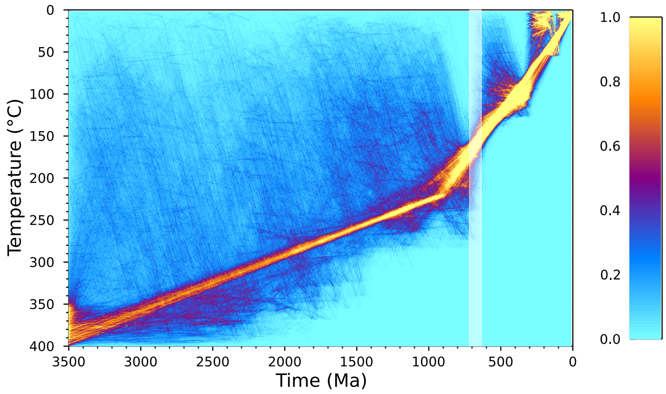


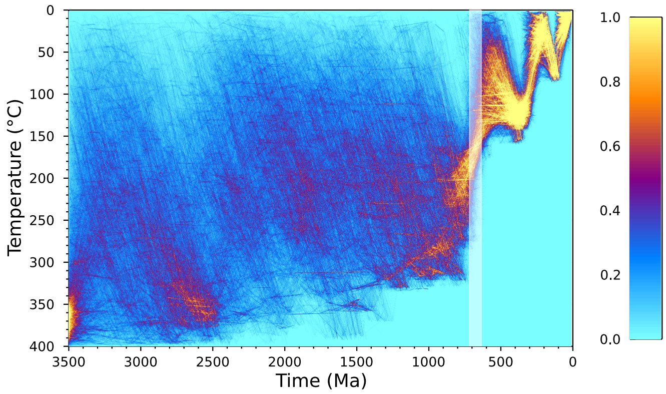
Figure 1: Schematic time-temperature plot showing three cooling curves of decreasing cooling rate from high to low temperature. In thermochronological inversions typically comprising a group of possible solutions, variable rate is a source of uncertainty and cooling onset is mostly controlled by data sensitivity (i.e., how well the model t–T path resolves some true cooling signal). For example, if the true total cooling magnitude is 200°C, and the data are only sensitive to temperatures $\leq$ 100°C, then the apparent cooling onset with be temporally biased by the difference in time between the true cooling onset and data sensitivity onset, proportional to the slope of the cooling curve. Thus in this scenario, cooling onset would only be accurate for near instantaneous cooling and would be highly inaccurate for situations involving slow cooling—more similar to that expected in a cratonic setting like Minnesota. Moreover, if chronometer data are low sensitivity then direct bias can be introduced by t–T constraint box arrangement portraying a seemingly well-resolved but inaccurate onset of cooling. Refer to McDannell and Keller (2022) for further discussion. It is our opinion that cooling onset is difficult to interpret and it is arguably less important than the time of 'peak cooling' for an overall cooling signature—when the first derivative of the cooling curve is maximized. The time of peak cooling is the same for all cooling curves shown here, as is the time of the true cooling event, yet with dramatically different times of "cooling onset".

4.3 Continuous spread of ages as a function of eU

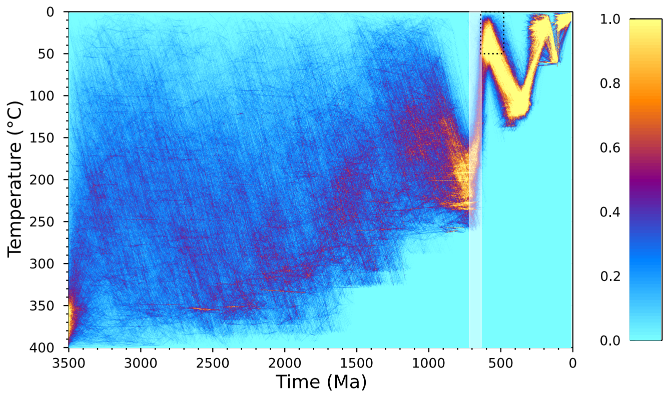
Fox et al. also discussed an aspect of the measured ZHe data that directly plays into thermal history recovery—the impact of the spread in zircon eU—and if the spread is narrow, sensitivity is limited and modelled histories are more uncertain (their fig. 6). This was also reviewed broadly in McDannell and Keller (2022); see their supplementary material. Fox et al. stated "***Many ages need to be sampled*** *in order to accurately capture the spread in ages over a specific [eU] bin*" and also said (line 295): "*The need to accurately capture spread are especially important if ages need to be averaged within [eU] bins to find acceptable paths as the uncertainty for the mean age is determined by the standard deviation.*" We would argue that their findings actually make a clear and obvious argument against binning ages by eU and averaging them in the first place. The need to capture the spread in ages supports collection of more ZHe data, not less by arbitrary means. The practice of eU binning and averaging is increasingly common but it is an ad hoc attempt to circumvent other statistical limitations (see McDannell et al., 2022b). Therefore, if eU binning is performed, the assertion that thermochronometer data are inherently "low resolution" is an oversimplification and without merit—since a natural outcome of averaging is information loss. All thermochronometers have fundamental limits on t–T resolution, which is the primary reason to apply *multiple* thermochronometers in deep time (McDannell et al., 2019; McDannell and Flowers, 2020).



(a) Canonical ZRDAAM Minnesota inversion without geologic constraints. **250,000** burn-in iterations and 250,000 post-burn-in iterations.



(b) Canonical ZRDAAM Minnesota inversion without geologic constraints. **350,000** burn-in iterations and 250,000 post-burn-in iterations.



(c) Canonical ZRDAAM Minnesota inversion with near-surface constraint at 560 ± 80 Ma between 0–50°C (black dashed box).

Figure 2: Inversion results for the Minnesota zircon (U–Th)/He data using `Thermochron.jl` and the canonical ZRDAAM kinetics. Cryogenian cooling is a consistent signal in all models. This is less clear in panel (a) due to incomplete burn-in; note the similarity with the Fox et al. QTQt models. Relative probability is proportional to path density, where warmer colors and higher saturation indicate more thermal histories pass through that region of t–T space (i.e., higher marginal posterior probability). The color scale is the normalized path density (minimum value of 0 is equal to no paths, and a maximum value of 1 is equal to the upper 95th percentile of path density). Except for panel (b), the Markov chain was run for 500,000 total iterations with a burn-in of 250,000 iterations. The prior was 400–0°C and 3500–0 Ma with a maximum allowed heating/cooling rate of 10°C/Myr (time step of 10 Myr). The modern surface temperature was allowed to be 0–10°C and the high-temperature starting condition was 400–350°C. White bar in each panel represents the Cryogenian Snowball Earth period from 717–635 Ma. QTQt plotting script is available at: `https://github.com/OpenThermochronology/QTQtPlot`.

5 Bayesian MCMC inversion tests

Here we show new models from a thermal history inversion code: `Thermochron.jl` (Keller et al., 2022), that utilizes a (transdimensional) Markov chain Monte Carlo algorithm similar to QTQt. The code is publicly available as a registered Julia package on OSF (`https://doi.org/10.17605/osf.io/wq2U5`) or Github at `https://github.com/OpenThermochronology`. Thermochron.jl currently only inverts the zircon (U–Th)/He system but is still in development with other thermochronometers being added. The code utilizes a 1-D Crank-Nicholson finite difference diffusion model and the published Guenthner et al. (2013) ZRDAAM kinetics. We present inversions that implement the same kinetic model variants presented in the Fox et al. manuscript with changes to the amorphous frequency factor. We focus on the canonical ZRDAAM and the low amorphous frequency factor model shown in their figure 5C, since that model exhibited the most apparent differences with respect to their normal ZRDAAM inversion. Inversions are shown with and without a geologic constraint. The usage of geologic/other information were minimized to align somewhat with the models presented in the preprint—yet we wanted to determine if the thermal histories are more consistent overall despite the kinetic model changes. A single Cambrian unconformity was either omitted or enforced in the model at 560 ± 80 Ma between 0–50°C. Cambrian and Ordovician rocks are present in Minnesota and the size of the constraint box is set conservatively small in time when compared to the other models shown without boxes (i.e., those models show cooling to surface temps. over a broader time interval—similar to the model that did not have a Cambrian constraint discussed in McDannell et al. 2022a).

5.1 Date uncertainty sampling

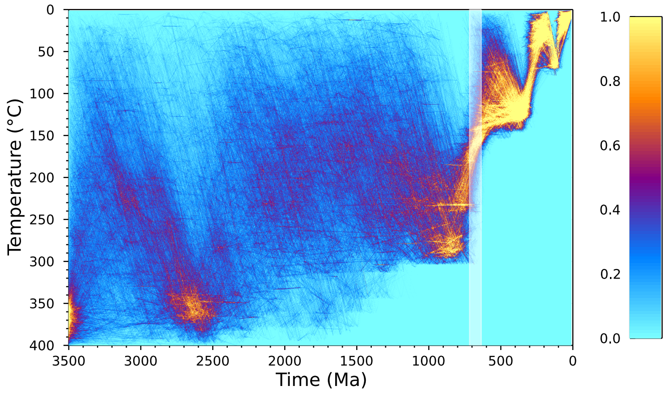
We allowed date uncertainties to be resampled (i.e., confidence in the derived uncorrected age but not the total uncertainty on that age), while making the same kinetic model changes as in the Fox et al. paper. They briefly mention age uncertainty treatment in QTQt (lines 268–281) and in that paragraph: "*Either additional uncertainty can be assigned to the measurements by resampling a scaling factor (> 1) that multiplies the input errors. This tends to allow the predicted age-[eU] relationship to pass through the observed data+resampled uncertainty. Or, alternatively, the thermal history can be adjusted to change the predicted age-[eU] relationship to try and ensure that the predictions fit the data, at least to within the error.*" We prefer investigating the data uncertainties because in general little is known a priori about the total size of the errors associated with ZHe dates—except that the observed reproducibility of ZHe dates rarely approaches the analytical precision. Known factors such as U-Th zoning, grain geometry estimation/alpha-ejection correction uncertainty (see Reiners et al., 2017 for summary), and radiation damage zoning cause excess age dispersion (Anderson et al., 2020). Currently, radiation damage models assume uniform kinetics. The model misfit between observed and predicted ages cannot be attributed only to the kinetic model because the kinetic model cannot explain the overdispersion of grains with identical histories and eU. Both kinetic model uncertainty and a wide range of geological and analytical uncertainties contribute to the total misfit between model ages and analytical ages. However, dispersion observed for grains of equivalent eU show that much of the misfit is a result of the latter processes (see Minnesota zircons for an example of this). Resampling the total date uncertainties can accommodate both kinetic and other unknown or poorly characterized sources of dispersion.

We handled date uncertainties differently than in QTQt or in the McDannell et al. (2022a) inversions (the latter utilized the 'scaling factor' mentioned by Fox et al.—except for the MRVT dataset; see text below). The zircon (U–Th)/He date uncertainty (`AnalyticalSigma`) was set to 10% for most grains (50% errors highest eU grains) and the `ModelUncertainty` was set to 25 Myr, which is not well known as it depends on annealing/diffusion parameters and decay constants etc—but it is certainly non-zero. A Simulated Annealing approach (SA; e.g., Kirkpatrick et al. 1983; van Laarhoven and Aarts, 1987) was used to increase the rate at which the Markov chain explores the probability space during burn-in, by adding an additional uncertainty term (`InitialUncertainty`; 35 Myr), which slowly decays to 0 with a decay constant of λ over the burn-in period[†]. As a result, SA initially makes it more likely to accept an unfavorable solution, but then slowly decreases the probability of accepting lower likelihood solutions as

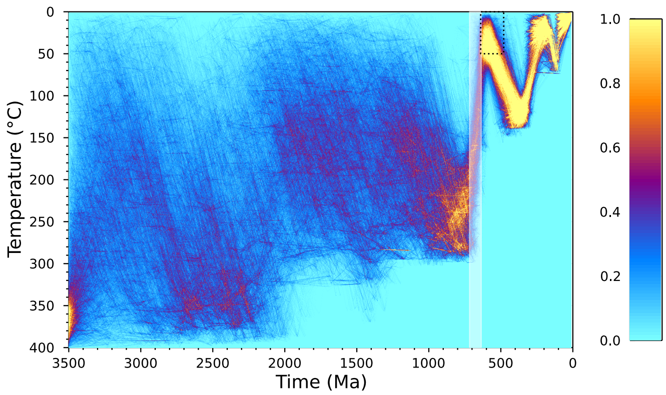
[†]The `AnalyticalSigma` was added in quadrature to the `AnnealingSigma` to yield `Sigma`, which is defined as the total date uncertainty. `Sigma = sqrt(AnalyticalSigma`^{2} `+ AnnealingSigma`^{2}`)`; where, `AnnealingSigma = InitialUncertainty * exp(-`λ`) + ModelUncertainty`. So for example, the oldest input MRVT uncorrected grain age was 770 ± 77 Ma. The starting uncertainty was ± 97.6 Ma [given as: sqrt((35+25)^2 + 77^2)] that decayed to ± 80.9 Ma [given as: sqrt((35*exp(-10)+25)^2 + 77^2)] by the end of burn-in, which is similar in initial error magnitude to the Empirical Bayes error resampling approach used in McDannell et al. (2022a) for the Minnesota example (i.e., oldest grain age input as 770 ± 100 Ma).

the model space is explored. Since it is necessary to temporarily accept a less favorable solution to escape a local optimum (and ultimately find the global optimum), accepting less likely solutions early in the inversion perhaps counterintuitively accelerates convergence by allowing for a more extensive search of the parameter space for the global optimum. As a result, SA can speed up convergence to the stationary t–T path distribution with a shorter burn-in. In contrast, in a standard MCMC inversion without SA, low likelihood solutions have an equal probability of being accepted at any time during the burn-in. Given sufficient burn-in, this also results in a thorough global search but may require a longer burn-in to achieve convergence on the global optimum and thus stationarity.

This SA approach should not be confused either with the Hierarchical Bayes uncertainty resampling currently supported by QTQt, or the Empirical Bayes uncertainty resampling (e.g., Malinverno and Briggs, 2004) that can be applied to ZHe data prior to either QTQt or Thermochron.jl inversions. Hierarchical uncertainty resampling in QTQt allows independent, random scaling of each date error, which will not necessarily assist in convergence on the stationary distribution. Hierarchical and Empirical Bayes resampling may also change the posterior distribution if the date uncertainties are either under- or overestimated. Ideally, Hierarchical and Empirical Bayes resampling both increase the accuracy of the posterior (i.e., make the stationary distribution better reflect reality). Whereas, SA does not increase accuracy but it will help find the posterior distribution more quickly and can be combined with forms of Hierarchical or Empirical Bayes resampling.



(a) Low amorphous frequency factor Minnesota inversion without geologic constraints.



(b) Low amorphous frequency factor Minnesota inversion with near-surface constraint at 560 ± 80 Ma between 0–50°C (black dashed box).

Figure 3: Inversion results for the Minnesota zircons using `Thermochron.jl` and the low amorphous frequency factor kinetics provided in the Fox et al. preprint. The Markov chain was run for 500,000 total iterations with a burn-in of 250,000 iterations. All other models parameters were the same as those in figure 2. We either omitted or enforced a single unconformity constraint in the model at 560 ± 80 Ma between 0–50°C.

5.2 Inversion results

Results demonstrate that there are no discernible differences (figs. 2 and 3) for parts of the inverted thermal histories with greater thermochronological sensitivity using the published ZRDAAM kinetics (figs. 2b and 2c) or the low amorphous frequency factor kinetics (figs. 3a and 3b). We recovered essentially the same thermal histories for each kinetic model variant with some expected, but minor, differences in the predicted vs. observed ZHe dates (fig. 4). Thermal histories were accepted that reach surface temperatures in late Precambrian/Cambrian time (figs. 2a and 3a), but their likelihood is lower because the data lack sensitivity to cooler temperatures, and simpler histories explain the data nearly as well. That was also a feature found to some degree in the Minnesota thermal history published in McDannell et al. (2022a; fig. 2C) that disappeared with applied geologic information (see McDannell et al. 2022a; fig. S1). Inadequate burn-in for the model in figure 2a produced a simple linear (but multimodal) high probability t–T region that was better resolved with a longer burn-in of 350,000 iterations (fig. 2b). Note that posterior probability behavior similar to this is present in all of the Fox et al. QTQt inversions. The approximate Cambrian surface constraint is necessary to moderate overly simplistic linear cooling posterior t–T paths spanning the late Neoproterozic to early Phanerozoic. The Minnesota inversions shown here are able to generally reproduce those shown in McDannell et al. (2022a); here excluding apatite (U–Th)/He data.

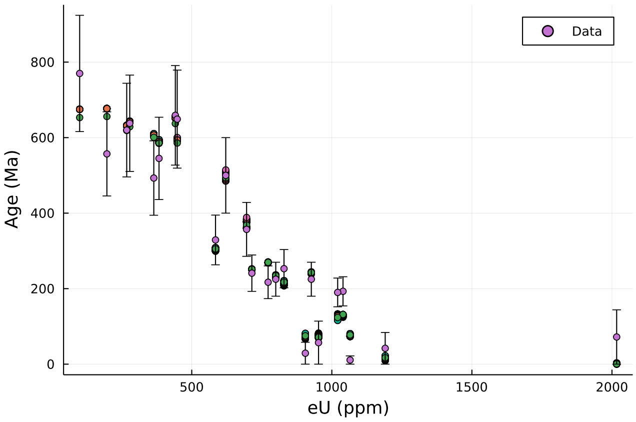
The Cambrian geologic constraint improves recovery/resolution of the late Neoproterozic-early Paleozoic thermal history for both kinetic variants (figs. 2c and 3b). The Phanerozoic portion of the model reproduces the Phanerozoic geologic record for Minnesota (Jirsa et al., 2011). We acknowledge that there are differences in the thermal histories for the pre-1200 Ma history for the canonical ZRDAAM and the low amorphous frequency factor models. The amount of Neoproterozoic heating allowed in the low-frequency-factor models is ∼30–40 °C hotter than the conventional ZRDAAM model, but this varies depending on kinetics, burn-in length, and trade-offs in time and temperature; compare figure 2b, figure 2c, and figure 3a near 1000–700 Ma. It may be that the low amorphous frequency factor kinetics produce unrealistically high temperatures required to reset the lowest damage (low-eU) zircons, since the late Paleoproterozoic was the last time MRVT basement underwent local magmatism and metamorphic temperatures of ∼300–350°C (e.g., Goldich, 1970; Bauer et al., 2011), although the complex regional geological evolution is still coming into focus (e.g., Southwick, 2014). The zircons are nonetheless thermally reset, regardless of the differences in heating magnitude between models. As Fox et al. stated (lines 301–302): "*The large uncertainties on the parameters controlling helium diffusion in zircon and the dramatic impact this has on temperature sensitivity highlights that this is important to consider*." The models we have shown here exhibit subtle differences in the recovered thermal histories, but overall they are very similar where the data have t–T sensitivity, which is reinforced when a single approximated geologic constraint is added.

Cryogenian cooling is consistently present in all of the inversions

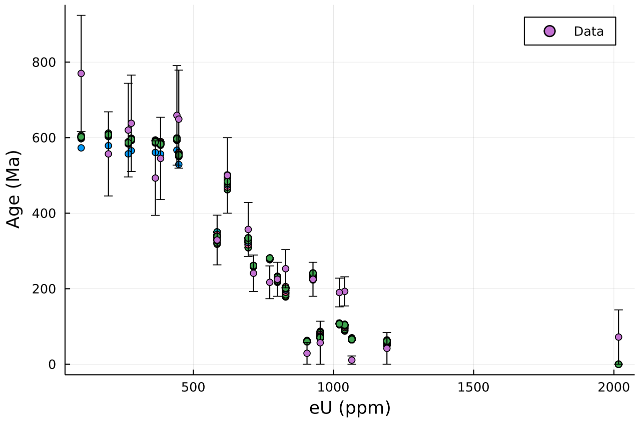
While the ZRDAAM kinetic calibration of Guenthner et al. (2013) is not perfect, the conclusions of Fox et al. may be overstated with respect to the effects of kinetic uncertainties on inverted thermal histories. That is not to say that more laboratory diffusion experiments on zircon should not be done—they most certainty should be performed. The authors provide an innovative solution to better incorporate estimates of kinetic model uncertainty into t–T inversions and this avenue is definitely worth pursuing in ongoing work. The authors may argue that some of the points addressed herein are outside the scope of their original manuscript, but it is one thing for their paper to discuss a realistic outlook on the precision and accuracy of kinetic models, and another to discuss those concepts for a single deep-time example—in our opinion, this results in a misleading framing of the current issues and their broader applicability. Hopefully this comment will stimulate further conversation on these important topics.

Kind regards,

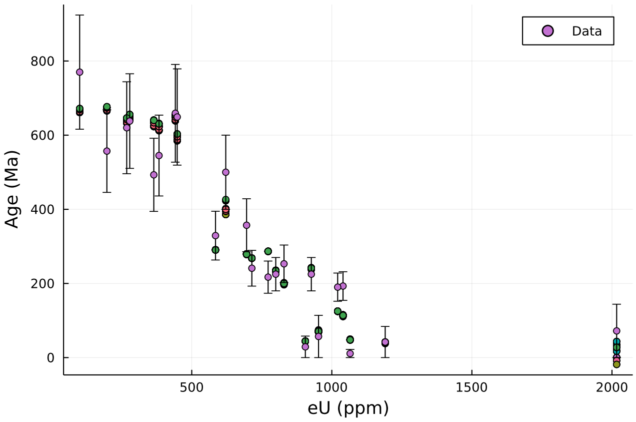
K. McDannell



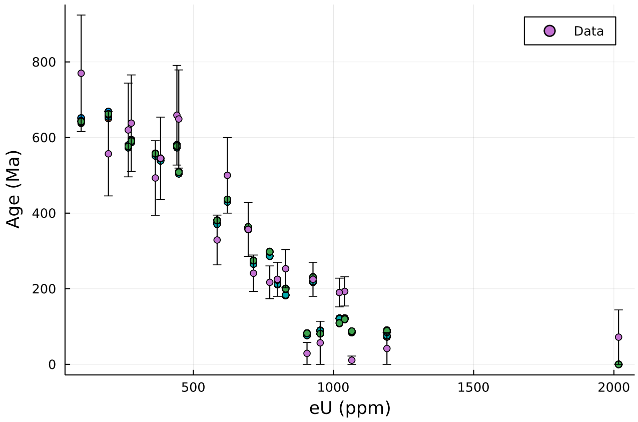
(a) Observed versus model predicted dates with respect to eU for ZRDAAM inversion without geologic constraint. 250,000 iteration burn-in.



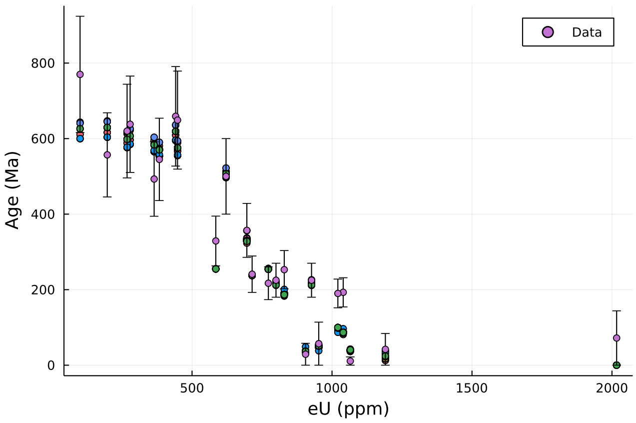
(b) Observed versus model predicted dates with respect to eU for ZRDAAM inversion without geologic constraint. 350,000 iteration burn-in.



(c) Observed versus model predicted dates with respect to eU for ZRDAAM inversion with geologic constraint.



(d) Observed versus model predicted dates with respect to eU for low amorphous frequency factor inversion without geologic constraint.



(e) Observed versus model predicted dates with respect to eU for low amorphous frequency factor inversion with geologic constraint.

Figure 4: Predicted zircon (U–Th)/He date-eU trends for the `Thermochron.jl` inversions. Purple points are input uncorrected data shown with uncertainty (`AnalyticalSigma`*2; for plotting purposes only). Other colored points are the predicted dates from the posterior distribution of the accepted t–T paths.

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