EGUsphere, author comment AC2
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Reply on RC2

Peter E. Martin et al.

Author comment on "Calculation of uncertainty in the (U–Th)□/□He system" by Peter E. Martin et al., EGUsphere, https://doi.org/10.5194/egusphere-2022-299-AC2, 2022

We would like to thank Dr. Ickert for his review; we respond to his feedback in-line below, using **bold** to easily differentiate our response.

This manuscript presents an algorithm for determining U-Th-Sm/He dates in accessory minerals and then derives uncertainty propagation equations for them, combining uncertainties in measurements of nuclide amounts and geometric correction factors. They also introduce a Monte Carlo method and compare the two. These algorithms are implemented in a python package hosted on zenodo.

A consistent set of uncertainty propagation equations for the community is a welcome addition to the literature, although it is unlikely that it will strongly affect science derived from the measurements due to pervasive overdispersion.

We generally agree with this assessment regarding current and archival data. However, by accurately constraining uncertainty (or, more specifically, the probability distribution) of an analysis, we can also accurately constrain the amount and distribution of overdispersion present in a given dataset to better understand the causes. This work also has the potential to future-proof the field as the technique is applied to increasingly challenging phases and time periods (both deep time and unusually young samples) where analytical uncertainties may become more significant.

I've had the opportunity to read the review by Pieter Vermeesch prior to writing this, and that saves me a lot of time writing my review because I came to basically the same conclusions as him. I don't think it's necessary for me to state specifically on which points I agree, but one that affects the manuscript substantially is the suggestion to cut down the length. I agree that section five can be completely removed. I don't think it's necessary for the authors to include log functions to the analytical solutions, but I agree that it would be a superior technique.

Section 5 – the entire discussion of the manuscript – is a fundamental part of this paper, just as the discussion is critical for any manuscript. This section shows the influence of input uncertainties on output uncertainties, is potentially critical for readers who do not have a strong foundation in the mathematical concepts presented earlier in the paper (based on experience with hundreds of (U-Th)/He data users at all levels), and shows the implications for real data. A clear example applying mathematical concepts is often the bridge to

understanding for anyone struggling to follow a purely conceptual discussion. It was our understanding that Geochronology is a journal intended for exactly this type of contribution. However, we do appreciate the suggestion that Section 5 can be tightened up, and we will revise the manuscript to keep Section 5 appropriately terse and present some of the less impactful discussion points (e.g. MC vs linear uncertainty propagation) to the appendices.

What I think would be very useful is a comparison of before/after of typical analyses from the authors lab. A few representative datasets would be just fine. I think this would be of great value in showing readers whether this approach changes assigned uncertainties in any substantial way. Maybe it doesn't, but that's not necessarily a bad thing.

We are not sure exactly what this suggestion entails? Since there is currently no generally accepted method for uncertainty propagation in (U-Th)/He dating, there is not really anything to compare against. While we could provide a comparison between the uncertainties assigned to the data in CU TRaIL prior to the development of this method, this comparison would be highly specific to our lab and would likely not be predictive of what other labs would observe if they made such a comparison.

I think it's a missed opportunity somewhat to not assess the accuracy of assigned uncertainties in the U-Th-Sm, and the He analyses. I appreciate that the authors have carved the manuscript such that this is "out of scope" (which is their prerogative), but the brief comment that tracers are often added by pipetting (without discussing the implications of adding a spike isotope using a technique with such a high variability) suggests to me that the radionuclide measurements may be underestimated. Not to mention that the treatment of under/over spiking and blank subtraction (to name a couple), in my experience, are dealt with in a highly variable way by different people in the U-Th-Sm/He community. I guess that leaves space for the next paper!

We generally agree that including uncertainty analyses for the component data (He, U-Th-Sm, and Ft) would be nice to have in the literature; the challenge, as mentioned in this comment, is that the techniques for these measurements are not consistent between labs. Such a discussion would therefore necessarily not be globally applicable and we do consider it beyond the scope of this paper. And including this discussion here would likely double or triple the length of the paper, which, as acknowledged by both reviewers, is already long.

I have a few shorter comments below:

L9: What quantities are ^{4}He and "radionuclide" here. Are they amounts, concentrations….? Please briefly define F_T in the abstract for a non-specialist, particularly because it's referred to as particularly important later in the abstract.

For the abstract, this is more of a general statement since a date can be calculated using either concentrations or amounts.
We agree that we should define Ft in the abstract, and will make this change during revisions.

L11: Is this relative or absolute uncertainty?

These are relative input uncertainties; we will clarify this in revision.

L15: Again, is this concentration?

These calculations were done with amount instead of concentration, but this isn't

a critical distinction given that the conversion to concentration has a common denominator for He and U-Th-Sm, and is therefore factored out in date calculation.

L15: What is the confidence level for these estimates? 95%? 2sigma?

The uncertainties in the abstract are quoted at 1-sigma; we will clarify this.

L34: I assume that by "kinetic" the authors mean diffusion kinetics.

Yes, we are referring to diffusion kinetics, and will clarify.

L76: "ppm" is, in general, ambiguous and best practice is that it should be avoided. I appreciate that there is an implicit convention in some geochemical subfields that it refers only to μg/g, but it is not always the case and there is no disadvantage to being explicit and using the SI-consistent μg/g.

This is a good point. We are referring to ppm by mass, so can make this change throughout the manuscript.

L80: "sector" should say "magnetic sector"

Yes, this is a good clarification.

L81: The technique is called "isotope dilution" not "isotope spike".

We will correct this.

L82: I'm not sure what "ratioed mass spectrometric measurements" are?

We are referring to ratio measurements (as opposed to absolute counts or voltages), and will clarify this.

L103-104: It's not clear to me that this is true. For example, if a mixed U-Th-Sm tracer is used and the mass of spike solution is relatively small (which is usually the case), the uncertainty in the amount of spike added (which propagates directly onto the amount of U, Th, and Sm calculated) will be relatively large and since the tracer is added as a mixture, that component will be highly correlated. It takes special care to get weighing errors to less than 1%, and with small amounts of spike they can easily be in the 5-10% range. When pipetting without weighing (which is what is implied here) the problem can be much worse. Pipetting consistency can vary, for sure, but for 25 μl the relative standard deviation on masses dispensed can be 3-5%, which translates directly to a 3-5% uncertainty on the measured quantities. This seems like it should be large enough to matter?

We think this is likely true for CU TRaIL based on our procedures and observed reproducibility, but correlated uncertainty associated with spiking procedures could be significant depending on the exact procedure used. We will add language to this effect and note that this may need to be assessed on a per lab basis.

L117: 2-9% in what? The Ft correction or the final date? And is this a bias (e.g., the technical definition of "error") or additional uncertainty on the date?

We will clarify this point—we are referring to uncertainty in the Ft correction, which will result in increased date uncertainty.

L131: Here and elsewhere the word "variance" is used. It's unclear as to whether this is referring to a moment of the gaussian distribution or as a casual synonym for uncertainty or data scatter.

Variance is explicitly not a parameter related to the gaussian distribution, but rather the formal term for "data scatter" (specifically, the expected squared deviation of a random variable from the mean) within any distribution. We used it here and elsewhere with the intention of being agnostic about the probability distribution reflected by an observed dataset while also using the formal language for scatter in a dataset. We will clarify this in the manuscript.

L366: A Th/U (by mass) ratio of 1.25 is *not* typical of zircon, it is unusually high. Looking at the georoc database of zircon compositions, after doing some data culling, the median value is about 0.6 (mean = 0.8). That sounds much more realistic to me than 1.25.

Thanks for this. This is a typo we discovered after submission; 1.25 is meant to be in reference to a typical apatite and 0.6 is our FCT number, which we applied to the zircon in this work. We will correct this during revisions.

L420: This statement should be justified or referenced, or else removed. It sounds a little bit like it is underestimating the math and stats skills of typical geochronologists.

Thanks for this reaction. We will modify this statement to "Figure 4 illustrates examples of combining uncertainties with differing magnitudes in quadrature." Hopefully this clarifies that, rather than an implicit low appraisal of most geochronologists' math/stats skills, this paragraph is meant as a simple exercise to build understanding for less advanced readers (e.g. undergraduates or early graduate students), and to prompt the memories for more advanced readers.