Comment on egusphere-2022-299
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Referee 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-RC1, 2022

This paper discusses the error propagation of (U-Th)/He data. Its introduction claims that “the formal analytical uncertainty in (U-Th)/He dates has never been thoroughly assessed”. I have three comments about this statement:

- I am sure that the error propagation of the (U-Th)/He method has been worked out before, and probably several times. In fact, I have done so myself, and even implemented it in a publicly accessible computer program: https://ucl.ac.uk/~ucfbpve/heliocalc/.

- One probable reason why nobody published the error propagation formulas for the (U-Th)/He method is the overdispersion that characterises most (U-Th)/He datasets: the scatter of several aliquots from the same samples usually exceeds the precision of the data, by a lot. So, in a sense, the analytical uncertainties are irrelevant. The interplay between analytical uncertainty and overdispersion is discussed by Vermeesch (2010, doi:10.1016/j.chemgeo.2010.01.002), who also covers some aspects of the error propagation problem.

- A second reason why error propagation hasn't been discussed much is that it is next to impossible to quantify the analytical uncertainty of the alpha ejection correction, which is one of the main sources of uncertainty in (U-Th)/He dating. Geochronologists slap a nominal uncertainty on this correction, which largely defeats the purpose of rigorous error propagation for the other variables. Unfortunately, the paper under consideration does not address this issue.
Despite these three caveats, I do not object to publishing the error propagation formulas in GChron. However, before this can happen the manuscript needs serious revision. The paper is far too long and can be shortened by at least 50%. I will make some specific suggestions for this later in this review.

The paper uses both standard error propagation and Monte Carlo (MC) simulation. I have two comments about this:

- According to the authors, the main advantage of the MC method is its ability to handle skewed error distributions. However, it would be easy to adjust the conventional error propagation to handle the observed skewness. This can be achieved by reformulating the error propagation formula in terms of the log of the variables (e.g., Section 5 of https://doi.org/10.5194/gchron-2-119-2020). Thus, the log of the age could be calculated as a function of the U, Th and He concentrations. An even better solution would be to use log-ratios. See Vermeesch (2010) for details. I am not sure how easy it would be to reformulate the paper and HeCalc code in terms of log(ratio) variables. If the authors find it too difficult, then I guess that the MC approach would be fine as an alternative.

- The actual main advantage of MC error propagation is not mentioned, namely its ability to handle non-Gaussian error distributions. This is particularly pertinent with regards to the alpha-ejection correction (i.e. the uncertainty of the alpha-retention factor Ft). Meesters and Dunai (2002, https://doi.org/10.1016/S0009-2541(01)00423-5) and Hourigan (2005, https://doi.org/10.1016/j.gca.2005.01.024) have shown that compositional zoning can strongly affect the fraction of ejected alpha particles. Matters are further complicated in the presence of broken grains, when the alpha ejection correction may result in overcorrection (Brown et al., 2013, https://doi.org/10.1016/j.gca.2013.05.041). Things are even more difficult for slowly cooled samples, in which alpha-ejection occurs synchronous with diffusive loss of helium. The dispersion caused by all these complexities is difficult to ascertain, but is likely non-Gaussian. The MC approach could be used to explore these effects. I’m not saying that the authors should do this in their paper (because I don’t want to make it even longer), but they should at least mention the possibility. Perhaps HeCalc could offer an interface to explore these effects?

Detailed comments:

Equations 4-10 are unnecessary. They are simply repeating Meesters and Dunai (2005,
Incidentally, I do not really see the point of using the Meesters and Dunai (2005) solution as a starting point for a Raphson-Newton algorithm anyway. Their direct solution is accurate to better than 0.1% for ages up to 500Ma, which covers all terrestrial applications of the (U-Th)/He method.

Equations 11 and 12 could be written more succinctly in matrix form.

Equations 14-18 all share the same denominator (which equals df/dt), which could be stored in a variable. All these equations could be put together into a single Jacobian matrix, or moved into the appendix.

Section 3.3.2 describes a method to choose the optimal number of MC iterations to derive a desired level of precision on the mean value. It just presents the well known “the square root of n” phenomenon, which I think is too trivial a result to occupy so much space (Figure 2 is certainly not necessary). It is also important to note that the square root of n rule only applies to the standard error of the mean. The standard error of the standard deviation (s) is given by s/sqrt(2n-2). I am mentioning this here because the uncertainty of the standard deviation is more relevant than that of the mean, which is never used in the remainder of the paper.

I installed HeCalc on my computer and am happy to confirm that it works. I have not extensively tested it though. I think that the presentation of HeCalc should take greater prominence in the paper. Of course, this will automatically happen if some of the remaining bulk is removed.

HeCalc requires that the user provide the uncertainties of the alpha-retention factors 238Ft, 235Ft, 232Ft and 147Ft. However, the paper does not explain how these uncertainties should be obtained. A nominal 5% uncertainty is used in later examples, without proper justification.

HeCalc also requires that the user specify the error correlations between the different parameters. However, it does not discuss how to estimate those correlations. Does the CU TRail database specify them?

Minor comment: the paper (and HeCalc) use the awkward convention to report MC uncertainties as “68% confidence intervals”. I understand where this comes from: a 1-sigma interval around the mean of a normal distribution covers 68% of that distribution. However, uncertainties are usually reported either as standard errors or as 95% confidence intervals. If the authors want to compare their analytical results with the MC simulations, then a 95% confidence interval would be more elegant.
Section 5 can be nearly completely removed. The most interesting part of this section is the finding that parent concentrations are a greater contributor to the uncertainty budget than the helium concentrations. This finding could be reported much more succinctly.

According to lines 421-423: “when combining uncertainties with equal magnitude, the resulting uncertainty will be only ~1.4 times larger than the input, rather than twice as large as might be expected.” Here the authors underestimate the reader. I am certain that the vast majority of geochronologists are familiar with the quadratic addition of uncertainties. Consequently this sentence, as well as the preceding paragraph and Figure 4, can be safely removed.

The paper attributes the reduction of analytical uncertainty with increasing date to the "roll over" of the exponential decay function. This may be correct but is largely irrelevant to real world applications. The observed reduction only expresses itself at >1 Ga, while the vast majority of published (U-Th)/He dates are <200 Ma. At young ages, the helium age equation is linear to a good approximation (https://doi.org/10.1016/j.chemgeo.2008.01.027). Note, however, that the fixed uncertainty of the helium measurements shown in Figure 3 is not realistic: older samples will tend to contain more helium, which can be measured more precisely. This will also cause a reduction of analytical uncertainty, even for Cenozoic samples.

In section 5.2, the authors introduce a new definition for skewness. This is a very bad idea. There already exists enough confusion in the geological community about basic statistical concepts. It would be unwise to add to the confusion by redefining widely accepted terms such as skewness. At this point I would like to reiterate the fact that the approximately lognormal uncertainty distribution of the dates could easily be captured analytically by recasting the equations as a function of the log of the age. Simply referring to the percent uncertainty of the age would capture the uncertainty and the skewness with a single number.

Section 5.4 applies the algorithms to a database of ~3,600 (U-Th)/He dates. It is a shame that this database is not released along with the paper. It must be a treasure trove of useful information! Unfortunately, I don’t think that Section 5.4 is particularly interesting. It definitely doesn’t deserve seven manuscript pages, four pages and three figures (not counting sub-panels). However, Figure 11 does illustrate my comment at the start of this review effectively: the nominal uncertainty of the alpha-ejection correction dwarfs the other uncertainties, thereby defeating the purpose of the careful error propagation.

Lines 615-616: “a challenge to interpreting data with asymmetrical uncertainties is that no widely used inverse thermal history modeling software for (U-Th)/He data permits the input of asymmetrical uncertainty” I’m not sure how HeFTy handles the analytical uncertainty of (U-Th)/He data, but if I seem to recall that QTQt essentially inflates the uncertainties until they account for the overdispersion of the data. This means that the uncertainties are, effectively, ignored. HeFTy probably does something similar, because otherwise its formalised hypothesis tests would fail. Ideally, thermal history inversions should aim to predict the uncorrected (U-Th)/He dates, ignoring the alpha ejection
correction. As mentioned before, this is because alpha ejection occurs concurrently with thermal diffusion. So it is not a constant but a variable that depends on the thermal history (Meesters and Dunai, 2002).

Equations a1-a10 all have the same denominator. Storing this denominator in a variable would avoid a lot of duplicate text. You could then even put all these equations into a single concise Jacobian.

I apologise if this review comes across as overly critical. I think that this paper (and the HeCalc program) could serve a useful purpose. My opinions is that it would be greatly improved by trimming it down to the important parts. Perhaps the paper could be recast as one of GChron’s popular “Technical notes”? This would provide a nice way to present HeCalc to the world, whilst reviewing the error propagation problem.