Response to RC2 Comments

Barra Peak
March 31, 2025

RC2: The author provides a set of equations to calculate volume and surface area, which seems generally uncontroversial, as far as I can tell. The R code may be useful for some. Generally, the manuscript could be improved if it more clearly stated what measurements are actually required as input for each of the geometric cases, and if the equations were appropriately justified when they are introduced. As it is, there's insufficient discussion to justify some of the assumptions going into the equations, and many of the variables+equations are poorly explained or not explained at all.

AC: I appreciate the reviewers taking the time to provide detailed feedback on where they found the manuscript confusing and needing clarification. They have made many suggestions which once incorporated will greatly improve the manuscript. I agree with the majority of their criticisms and need for additional discussion of how the protocols presented in this manuscript differ from existing approaches in order to justify adoption of these protocols.

I am not opposed to including more explanation of the background equations used in the protocol described here and I agree that doing so would make the paper more accessible to a broader audience. However, to me, this feedback suggests that the reviewers and I may have different understandings about the purpose of a technical note paper and clarification of the intended purpose from the editor would be helpful prior to revisions. I agree completely with the need to better explain and justify how my proposed protocol differs from existing methods; however, I am not sure how much background explanation of existing equations and variables on which the method is based is needed. I wrote the original manuscript with the understanding that a technical note should be brief and targeted to a very specific methodological problem or advancement – e.g., something that in other cases might end up in the supplement of a paper framed around a geologic question and interpretation. Thus, my understanding of the intended audience of a technical note is other scientists who run into the same specific methodological problem—other thermochronologists conducting bulk-helium analyses on polished grain fragments. As such, I assumed the audience would have a common background regarding how geometric grain classifications are made and the justification for the use of general geometric equations for volume and surface area to describe these geometries such that rather than providing detailed explanation of existing equations, citation of the relevant literature (e.g., “Eq. 3 of Ketcham et al., 2011”) would be sufficient. The fact that both reviewers asked for more detail and discussion on this background shows my assumptions were wrong and suggests to me that they may have a different interpretation of the intent of a technical note. Editorial input about the intended purpose and audience of a technical note as well as clarification about length limits, would help me determine the best course for revisions and if a technical note is actually the best channel to share the methodological protocols presented here.

Other comments:

RC2: First, I would suggest that the author reconsider the use of “volume and derived value” in the title, which could be more informative if it specified, for example, “improved calculation of

volume, FT correction, and other derived values for polished zircon"… At the end of the day, the FT correction is what most readers are interested in.

AC: I agree, thank you for the suggestion.

RC2: Second, the manuscript would be much improved with greater discussion of the specifics of how the proposed calculations differ from previous protocols (e.g. in Lines 210-215). The equations are presented, but not much is done to demonstrate their superiority, besides Figure 2. Which cases lead to the large (95%) variation? It seems to be just a single grain or two? In what cases/geometries/grain sizes generally have minimal difference between the different protocols? Is it small grains that are particularly effected? or when very little of the grain is polished, or a lot of it is polished away?

AC: I agree that this would strengthen the manuscript. Notably, the conditions under which the different protocols are designed to apply are very different, with the Reiners et al. protocol limited to ellipsoid or tetragonal grains polished parallel to the c-axis and less than halfway through the grain. I agree that this is an important point that is missing from the current manuscript. A better Figure 2 can be used to address some of the specific questions raised by the reviewer regarding the impact of grain size and polishing depth rather than extensive additions to the text since it is my understanding that the text is already on the long side for a technical note. Editorial clarification on this would be appreciated.

To more fully assess the differences between protocols in cases when the Reiners et al. protocol is designed to be applicable, a comparison of a synthetic set of zircon data with a range of size, parent isotope concentrations, and polishing depths could be made. I did not include this previously as the conditions that satisfy the Reiners et al. protocol starting conditions apply to only a small subset of possible conditions, which is reflected in the real dataset presented and a main motivator for the development of the new protocol presented. Again, I realize this point is not clearly articulated in the present manuscript and needs to be more explicitly stated.

RC2: A histogram could be provided showing the % difference between the different protocols for each grain in the dataset. Is there a systematic skew towards overestimating or underestimating FT?

AC: I agree this could be a helpful addition to Figure 2; thank you for the suggestion.

RC2: Notably, Fig. 2 only shows that these protocol are different. But it's not immediately clear why, practically speaking, the additional complication of assigning grains to particular sub-classes of geometries and degrees of polishing based on limited 2D measurements from a polished mount wouldn't simply be introducing more assumptions and/or errors. I could certainly imagine how these detailed calculations here could be better - but I don't think that's necessarily the case, and the author needs to demonstrate that.

AC: I agree that further discussion and justification of this method compared to others is necessary. I think this would be done best using a synthetic dataset, similar to what was done in the He and Reiners (2022) paper. I address this further in subsequent responses.

RC2: For example, the author states that “The Reiners et al. method of accounting for FT corrections due to polishing, while frequently resulting in < 5 % difference, can also vary more significantly, likely due to simplifying assumptions made by this method regarding grain geometry, orientation, and depth of polishing.” The author should expand on this sentence and explicitly discuss those simplifying assumptions. How and when exactly do they vary so significantly? And most importantly, for many readers, the question is whether it is practical to move beyond those simplifying assumptions. It would be helpful if the author distinguished the specifics of the cases (e.g. the one with the 92% difference) that led to the large difference. Why and how are the approximations that are used here (particularly for the c-axis parallel cases) better/different than the simplifying assumptions used by others?

AC: I agree that more explicit discussion of the assumptions is needed. The Reiners et al. method assumes grains are polished parallel to the c-axis, polished less than halfway through the grain but greater than one alpha-stopping distance, and does not provide a set of corrections for grains with cylindrical geometries. Further, the Reiners et al. method makes simplifying assumptions about the degrees of symmetry in ellipsoidal grains and the number of terminations present for tetragonal grains. These assumptions are not met by the majority of the real grains and polishing conditions presented in the manuscript, suggesting that the Reiners et al. method should not be used to correct these grains. However, I agree the manuscript currently lacks further justification of this.

To fully show the improvement of the protocol presented here over the Reiners et al. method comparison between methods using a synthetic dataset can be added that covers a broader range of conditions than the real dataset.

RC2: Third, when polished perpendicular to the c-axis, the calculations would essentially be the same case as the fragmentation correction for grains with one end broken, which we discussed in a similar paper (He and Reiners, 2022). For these cases, I imagine the modified FT would be exactly the same as the protocol propose here?

AC: Yes, the approach is the same in which the polished fragment has an F_T correction equivalent to a whole crystal with length 2x the fragment length and I apologize for not citing this He and Reiners (2022) in regards to this approach. The revised manuscript will be updated with this citation.

The same approach is used for ellipsoidal and tetragonal grains polished parallel to the c-axis when more than half the original grain is removed except in these cases the relevant plane of symmetry is different and thus the axis modified by a factor of 2 is the b-axis in the case of ellipsoids and the a-axis in the case of tetragons.

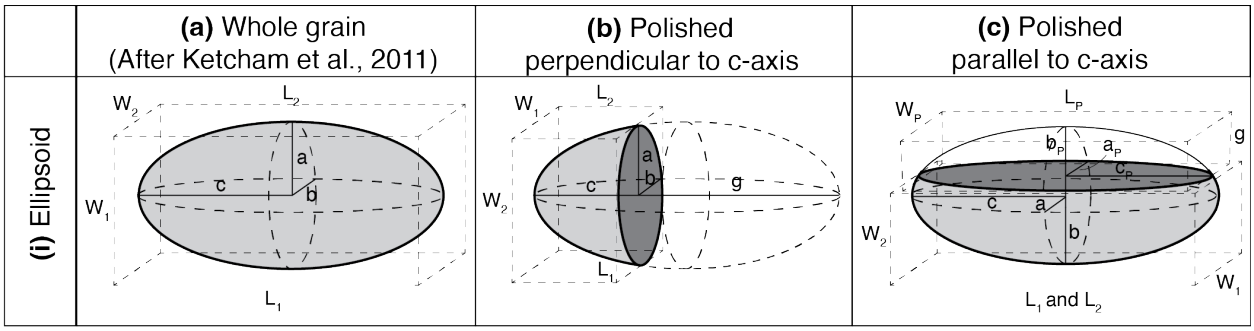
RC2: Finally, something additional that would be relevant to add in the discussion: the idea that the SA/V of polished grains can be used to modify FT corrections assumes that the polynomial function relating SA/V to FT is nearly identical for most geometries. But it is not entirely identical, and polished grains would deviate pretty far from ideal geometries used to determine the SA/V-FT functions.

AC: I agree that this is worth discussing. Revisions to Section 2 will reflect this.

Other comments:

RC2: It's not clear from Fig. 1 what the different labels (e.g. w1 wp) are referring to in many of the diagrams.

AC: Thank you for the feedback that this is unclear. W1, W2, L1, and L2 are the measurements made of the grain while a, b, c, r, and h refer to the axes, semi-axes, radius or height of the idealized geometry. The figure is meant to show visually how these relate to each other to compliment the mathematical relationships between measurements and geometric parameters given in Table 1. Sets of W1, L1 and W2, L2 measurements are made by rotating the grains 90° such that these measurements can also define a rectangular prism that surrounds the grain as in the example below. Does the example better confer the intended relationship? Measurements and parameters axes could also be color-coded to their respective labels.



RC2: What you call SA is not actually surface area - but rather something like the alpha-ejection-affected-surface area. I suggest using a subscript to clarify this (SA_α), or something similar, as it is can be confusing to readers. Note that in He and Reiners 2022, we called β_α =the ratio of alpha-ejection-affected surface area to volume.

AC: This is true, and this modification of "SA" from the true SA is explained in lines 68-69. I will clarify this modification of "SA" earlier in the manuscript.

The protocols proposed in the manuscript are based directly on the protocols of Ketcham et al. (2011) which uses SA to refer to alpha-ejection surface area (albeit assuming the entire grain surface area is an ejection surface) and equivalent spherical radius, R_S, defined as 3V/SA in the formulation of F_T rather than β_α. I adopted the same formulation of F_T and R_S terminology to be consistent with Ketcham et al. and to aid a reader who would likely be comparing directly between that and the protocols presented here (R_S was changed to R_{SV} reflecting reporting standards used at CU TRaIL to differentiate from R_{FT}). R_{SV} and R_{FT} are important values in their own right, as they are commonly reported as a description of grain size and used in thermal history modeling software programs. In the interest of not introducing even more variables, I elected to not reference β in the original manuscript, but I am happy to add reference to it since more readers may be familiar with it than R_S.

RC2: There should be more details about the test dataset: what was the measurement protocol? the range of grain sizes? how were the grains assigned into different geometries if they were already polished?

AC: Grain measurement protocol is partially described in Line 55. Grains fragments were easy to classify post-polishing once removed from the epoxy mount and viewed under a microscope as they looked like either half an ellipsoid, half a cylinder, or half a prismatic crystal with clear faces 90° to each other. These details will be added to the revised manuscript.