

Response to summary editor and reviewer comments

EC: The two reviewers were largely in agreement; they acknowledged the importance of the topic addressed in the manuscript, but pointed out that there was room for improvement in the presentation, including the wording, explanations of the equations/parameters, and comparison with the previous protocols. I generally agree with their comments and ask the authors to update their manuscript accordingly. If the two reviewers, who are experts in F_T calculations, felt that the approach was not explained well enough, it is likely that most readers will find it even more so. In response to the reviewer's comments, the authors proposed a comparison with the previous protocols using a synthetic dataset, which could be very useful information for potential users of the R script. Since the manuscript is a Technical Note, I think there is a limit to the number of pages, but I hope that the authors will incorporate this well into the manuscript, if necessary, using a supplement file, etc. - this is a personal expectation and not a requirement for acceptance. To conclude, I believe that this manuscript is potentially suitable for publication in the GChron journal after moderate revisions.

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 am grateful to the reviewers for taking the time to provide detailed feedback on where the manuscript needs improvement. The majority of the comments from the editor and both reviewers request additional clarification about the method presented in the manuscript, both in terms of how minerals are measured and classified, and the overall approach to F_T calculation. Both reviewers also requested more details regarding how the new protocol differs (or doesn't) from previously published methods that are used for comparison. I agree with the need for additional clarification, particularly for explaining the general approach to the new protocol. I have substantially reworded and added to the text in order to address these requests and correspondingly reorganized some of the content to keep the total length of the main text appropriate for a technical note. Equations now mainly appear in an Appendix (Appendix A), so that the main text of the manuscript is devoted to explanation of the approach and required measurements (Section 2) and evaluation of the new protocol (new Section 3). The main evaluation of the new protocol (new Section 3) has been updated to include comparisons using a large synthetic dataset. The comparisons using a real dataset that appeared in the original manuscript have also been revised and moved to Supplementary Text. The real dataset confirms results found with the synthetic dataset and now plays only a supporting role in the manuscript, making it appropriate for a supplement.

From the reviewer comments, it was clear that central components of how the new method is applied were not communicated in the original manuscript. Revisions to address specific comments and points of confusion are described below, but in general, the method is designed to calculate volume, alpha-ejection surface area, F_T , and all other values **after** grinding and polishing of grains has occurred and **only for the remaining grain fragment**. No attempt is made to apply "whole grain" values, as these would not be appropriate to combine with isotopic measurements made on the grain fragments anyway. Grain geometry classification is based on the grain fragment itself, not the original grain (although the two are often related – e.g., an ellipsoid grain typically becomes half an ellipsoid when polished). An expanded explanation of this approach is included in revisions to Section 2 and in Appendix A.

To address requests for more details and discussion of F_T comparisons between the new and existing protocols, I have reframed the method evaluation section (Section 3) around a new synthetic dataset containing 16128 synthetic polished and whole zircon (Table S1) that covers a much larger range of possible grains than the real dataset originally presented. Additions to Section 2 and Section 3 describe the Ketcham et al. and Reiners et al. methods that are used as points of comparison in more detail, as requested. In the process of making these revisions, I realized the Reiners et al. method had been incorrectly cited, and that has now been fixed.

Point-by-point reply to editor and reviewer comments

EC: Table S1: Length P - the long axis... --> Length P - the long axis...

Table S1: Width P... Typically indistinguishable... --> Width P... Typically indistinguishable...

AC: Thank you for pointing out these typos, they have been corrected in the revised tables.

RC1: From what I understand from your manuscript, your proposed approach will likely under- or overestimate the F_T value since you are using volume and surface area calculation of the polished grains for your calculation of F_T . The correct F_T value is dependent on both the original grain geometry and the resulting after polishing and only if half a grain is polished both will be similar. The resulting F_T value calculated with your approach will be smaller than the corresponding F_T value of the whole grain, in case polishing removes less than half of the grain. The opposite is in case more than half the grain is removed during polishing. Either show the difference to the correct value and state the limitation or implement the correct calculation.

AC: My approach is intended to provide an F_T correction for the grain fragment remaining after polishing rather than the whole original grain, regardless of how much of the grain remains. Since only U, Th, Sm, and He of the fragment are measured, applying an F_T correction based on the original, unpolished grain volume and surface area would be inappropriate without also somehow correcting these isotopic measurements to reflect the original whole grain morphology. Although this is theoretically mathematically feasible, the uncertainty associated with doing this – both quantifiable and unquantifiable – make it a worse option in my opinion than proceeding with just the direct measurements of the remaining fragment as done here. Based on this and other comments from both reviewers, it is clear to me that the basis of the approach – calculating values for the polished grain fragments, not the original whole grains – was not communicated effectively in the original manuscript. I have revised the Abstract, Introduction, and Section 2 to explicitly state that the protocol I am presenting is for polished grain fragments. I have also revised Figure 1 to illustrate how volume is calculated.

Line 15-18: “To address this issue, this paper presents a comprehensive protocol for calculating volume and alpha-ejection surface area for polished zircon grain fragments, from which additional data, including eU and F_T , are derived. This protocol is implemented after grains have been polished and in situ measurements have been made...”

Line 71-72: “To address the lack of a comprehensive approach to volume-derived data for polished zircon, this contribution presents a protocol and set of equations...”

Line 79-80: “The protocol presented here adapts existing approaches for determining whole-grain V, SA_α , and F_T for ground and polished grain fragments...”

Line 92-96: “In most cases, calculating these values [V, SA_α , F_T] is accomplished by adopting the same approach as He and Reiners (2022) in which the polished grain is treated as a crystal broken along a plane of symmetry such that V and SA_α of the polished fragment are half of a whole “assumed grain” created by reflecting the existing fragment across the plane of polishing (Fig. 1c). F_T of the fragment is thus equal to F_T of the assumed grain.”

Using the new synthetic dataset, I have also addressed the relationship between F_T for whole grains and polished grains in a new Figure 2 and related text:

Lines 185-191: “Across all geometries and grain sizes, the majority of grains exhibit expected changes in F_T with increasing grinding depth: polished F_T is greater than whole F_T up to 50 % grinding depth and polished F_T is less than whole F_T above 50 %. The smallest ellipsoid grains with the lowest aspect and width ratios are an exception to this pattern, which is likely related to partial removal of the remaining fragment’s alpha ejection rim at higher grinding depths. The largest grains exhibit the smallest differences between whole grain and polished grain F_T , but the difference increases once more than half the grain width is ground away as for other grain sizes (Fig. 2).”

RC1: Line 1,16: Specify what you mean with ‘derived value calculation’. Also, later you often say something like ‘other values’. Please make sure that you always specify the measurements you are referring to.

AC: Thank you for pointing out that “derived value” is vague and should be avoided or better defined. Here, I am using “derived values” in a manner similar to Flowers et al., (2022a) to refer to data or correction values such as F_T that are not directly measured but are derived from direct measurements, typically during “data reduction” steps of (U-Th)/He thermochronology workflows. Where appropriate, I have revised the text to specify the value being discussed. It is still sometimes necessary to refer to the category of values derived from direct measurements as a whole, so I have added explanation of “derived data” to the Introduction:

Lines 27 - 29: “((U-Th)/He thermochronology dates and associated data are derived from analytical measurements of parent and daughter isotopes and the volume (V) of the individual mineral grains analysed. These “derived data,” include alpha-ejection correction factors (F_T), F_T -equivalent spherical radius (R_{FT}), effective uranium (eU), and parent isotope concentrations...”

RC1: Line 8-17: You state that the proposed protocol is beneficial for in situ measurements (line 14) and later for bulk grain (e.g. line 16). Please state clearly which method (in-situ and/or bulk grain) would benefit.

AC: The protocol is beneficial for studies in which in-situ and bulk grain conventional (U-Th)/He thermochronology analyses are desired for the same grains. I have revised wording in the Abstract and Introduction to clarify this:

Lines 17- 19: “This protocol is implemented after grains have been polished and in situ measurements have been made and can be easily integrated into existing workflows for characterizing and measuring grains for conventional (U-Th)/He analysis.”

Lines 40-43: “However, many applications of (U-Th)/He thermochronology, such as detrital zircon applications, benefit from or require mounting and polishing crystals for in situ analyses to characterize chemical zonation, rare-earth element abundances, U-Pb or other geochronology data, etc. prior to (U-Th)/He analysis. Grinding and polishing grains to prepare them for additional analysis removes part of the grain...”

RC1: Line 49-50: You may want to reference to my approach using a set of orthogonal microscopic pictures to derive whole-grain geometries (Glotzbach et al. 2019 – Chemical Geology).

AC: Thank you for the suggestion; I have added this citation.

RC1: Line 48-58: Please clearly state what your approach is. Measuring only after mounting/polishing or, what I guess, two measurements are required before and after mounting/polishing.

AC: The approach uses one set of measurements made after the grains are polished. Section 2 has been revised to make this explicit:

Lines 79-81: “The protocol presented here adapts existing approaches for determining whole-grain V, SA_{α} , and F_T for ground and polished grain fragments. First, the polished grains are removed from the mounting medium and inspected and measured...”

RC1: Line 72: The word ‘irrelevant’ is somewhat misleading here, since the depth to which grains are polished is impacted V, SA and other related parameters and is not irrelevant. I guess you mean that it is easy to account/correct for.

AC: I agree better wording is needed here. In some cases, polishing depth is not needed since the volume and surface area of the remaining fragment can be calculated from measurements of the fragment alone. In other cases this is not possible and polishing depth is needed. I have revised Section 2 to better explain the different cases and updated Figure 1 to show how grinding depth is needed (or not) for calculation of geometric parameters.

Line 92-102: “In most cases, calculating these values is accomplished by adopting the same approach as He and Reiners (2022) in which the polished grain is treated as a crystal broken along a plane of symmetry such that V and

SA_α of the polished fragment are half of a whole “assumed grain” created by reflecting the existing fragment across the plane of polishing (Fig. 1c). F_T of the fragment is thus equal to F_T of the assumed grain. This is the approach used for all grains polished perpendicular to the c-axis or parallel to the c-axis and greater than halfway through the original c-axis perpendicular width of the grain (Fig 1c), which can be determined by visual inspection of the polished grain and does not require measurements of thickness pre-polishing. For grains polished parallel to the c-axis and less than halfway through the original width of the grain (again, determined by visual inspection of the grain post-polishing), a different approach to determining V and SA_α is used. In these cases, the original whole grain dimensions are estimated by combining the grain measurements with the grinding depth (g) determined by measurements of spherical glass beads mounted and polished alongside the grains.”

RC1: Line 74-77: See above, in case you measure individual grains before and after mounting/polishing this would not be required. Therefore I guess you are measuring only after mounting/polishing and derive the depth of polishing from the glass beads.

AC: Yes, grains are only measured after polishing. As noted above, Section 2 has been revised to clarify this.

RC1: Line 85-90: I do not fully understand how you can estimate the correct values of a and b for an ellipsoid (r for cylinder) in case more than half of the grain is polished away. The equations that you state will be minimum values for a and b (e.g. $b=W/2$).

AC: The geometric values calculated are not intended to reflect the original whole grain (whole ellipsoid, etc.), rather, they reflect the remaining fragment, which in most cases is well-approximated by a half ellipsoid, half cylinder, etc. (Figure 1, Lines 90 - 109). The semi-axes of the original whole grain and polishing depth are not used, which is reflected in revisions to Figure 1. Only in cases where the fragment morphology cannot be approximated as half an ideal geometry are the original grain dimensions estimated. To do this, grinding depth is used. I hope that this confusion is alleviated by revisions to clarify that the volume, alpha ejection surface area, F_T and other values calculated are only for the polished grain fragment, not the original whole grain.

Lines 92-111: “In most cases, calculating these values is accomplished by adopting the same approach as He and Reiners (2022) in which the polished grain is treated as a crystal broken along a plane of symmetry such that V and SA_α of the polished fragment are half of a whole “assumed grain” created by reflecting the existing fragment across the plane of polishing (Fig. 1c). F_T of the fragment is thus equal to F_T of the assumed grain. This is the approach used for all grains polished perpendicular to the c-axis or parallel to the c-axis and greater than halfway through the original c-axis perpendicular width of the grain (Fig 1c), which can be determined by visual inspection of the polished grain and does not require measurements of thickness pre-polishing. For grains polished parallel to the c-axis and less than halfway through the original width of the grain (again, determined by visual inspection of the grain post-polishing), a different approach to determining V and SA_α is used. In these cases, the original whole grain dimensions are estimated by combining the grain measurements with the grinding depth (g) determined by measurements of spherical glass beads mounted and polished alongside the grains. Polishing depth is calculated using Eq. (1) (Pickering et al., 2020) and measurements of the radius of the polished bead surface (r_{BP}) relative to the full bead radius (r_B).

$$g = r_B - \sqrt{r_B^2 - r_{BP}^2} \quad (1)$$

Uncertainty on g can be determined through duplicate measurements of multiple embedded beads scattered throughout the grain mount. The estimated whole grain dimensions are used to estimate V and SA_α for the whole original grain. To calculate V and SA_α of the remaining fragment, the V and SA_α of the removed portion of the grain are also estimated and subtracted from the estimated whole. V and SA_α of the removed portion are determined by treating removed portions of the crystals as half crystals of a whole assumed grain in the same manner as grains polished parallel to the c-axis and more than halfway through the original grain width (Fig. 1c). This calculation requires additional measurements of the polished grain surface: length (L_P) and width (W_P) of the polished face. In practice, L_P and W_P are often indistinguishable from L_1 and W_1 .”

In the case of grains that are originally cylinders polished parallel to the c-axis, I agree that the approximation for r and subsequent volume and surface area derivations presented in the original manuscript are not the best approximations possible. I have updated the approach to treat “cylinders” as prisms with ellipsoid pinacoid

terminations (or partial ellipsoids in the case of grains polished parallel to the c-axis, Fig. 1c) that can be described by semi-axes a and b.

Lines 294-317: “**A2. Cylinder volume and alpha-ejection surface area**

“Cylinders” can more accurately be represented as prisms with height (h) and ellipsoidal, rather than circular pinacoid terminations with semi-axes a and b (Fig. 1c). V and SA_α are calculated using the area of an ellipse (πab) and Ramanujan’s Formula for the perimeter of an ellipse (Eq. A5).

$$P_{\text{ellipse}} = \pi(a + b) \left[1 + \frac{3k}{10 + \sqrt{4 - 3k}} \right] \quad (\text{A5})$$

Semi-axes of the ellipsoid cross section are denoted as a and b, k is defined as $(a - b)^2 / (a + b)^2$, h is the height or length of the cylinder. Additionally, r is the original radius of the cylinder pre-polishing reconstructed as $r = \frac{(g + W_2 + W_1)}{4}$. The semi-axes are related to the 2D grain measurements and g depending on degree of polishing as given in Table 1. When the grain is polished perpendicular to the c-axis the grain is treated as half a symmetric prism broken perpendicular to the c-axis and V and SA_α are calculated using Eq. (A6) and (A7).

$$V = \pi abh \quad (\text{A6})$$

$$SA_\alpha = \pi ab + \pi(a + b) \left(1 + \frac{3k}{10 + \sqrt{4 - 3k}} \right) h \quad (\text{A7})$$

When the grain is polished parallel to the c-axis and more than halfway through the original width ($g > (W_2 + g)/2$), V and SA_α are calculated using Eq. (A8) and (A9) which treat the fragment as half of a cylinder:

$$V = \frac{1}{2} \pi abh \quad (\text{A8})$$

$$SA_\alpha = \pi ab + \frac{\pi(a+b)}{2} \left(1 + \frac{3k}{10 + \sqrt{4 - 3k}} \right) h \quad (\text{A9})$$

When the grain is polished parallel to the c-axis and less than halfway ($g < (W_2 + g)/2$), V and SA_α are calculated using Eq. (A10) and (A11) which combine estimated V and surface area of the whole original grain and the removed portion of the grain approximated as half a symmetric prism broken parallel to the c-axis.

$$V = \pi h \left(ab - \frac{1}{2} a_p b_p \right) \quad (\text{A10})$$

$$SA_\alpha = 2\pi \left(ab - \frac{1}{2} a_p b_p \right) + \pi h \left[(a + b) \left(1 + \frac{3k}{10 + \sqrt{4 - 3k}} \right) - \frac{1}{2} (a_p + b_p) \left(1 + \frac{3k_p}{10 + \sqrt{4 - 3k_p}} \right) \right] \quad (\text{A11})$$

RC1: Line 86: Specify what the ellipsoid coefficient is.

AC: The ellipsoid coefficient is a feature of Knud Thomsen’s formula to approximate ellipsoid surface area employed in Ketcham et al., (2011) and adapted here. A citation for this has been added to the text in Line 283.

RC1: Line 114-115: Same as for the ellipsoid does apply for a cylinder, it is not possible to correctly determine r when more than half the grain is gone. The equation that you are using $r = \min(W1, W2)$ will underestimate r. Why not using equation 1 to estimate the correct radius?

AC: I agree a better approach is possible. See above for revisions to the treatment of “cylindrical” grains by treating them as prisms with ellipsoidal terminations.

RC1: Line 158-186: It is unclear to me if you calculate the Ft for the whole grain or the mounted/polished grain. The Ft value of mounted/polished grains will in most cases be higher/lower than the theoretical value of the whole grain (similar only if exactly half the grain is removed).

AC: F_T is calculated using V and SA_α for the polished grain fragment only. As noted above, the manuscript has been revised to clarify this.

RC1: Line 187: Please add more details on how you did the comparison, are this read data or synthetic data and give details how the methods of Ketcham and Reiners differ from your approach.

AC: Thank you for the feedback that more details are needed. The data used in the original manuscript is a real dataset acquired for a detrital zircon sample; this is now contained in Supplementary Text. The main paper discusses comparisons using a synthetic dataset. How the synthetic dataset was generated is described in Lines 163-179:

“A synthetic dataset (Table S1) was used to evaluate the protocol and compare with existing approaches to calculating F_T values. The synthetic dataset was designed to test a range of original grain geometries, total grain sizes, grinding and polishing orientations, and grinding depths greater than the maximum average zircon alpha stopping distance ($> \sim 18.5 \mu\text{m}$; Ketcham et al., 2011). Total grain size was defined by a combination of “size” corresponding to the c-axis parallel length – generally the longest grain axis corresponding to grain length measurements L_1 and L_2 , “width ratio” between the two c-axis perpendicular grain lengths (corresponding to a and b crystallographic axes and grain width measurements W_1 and W_2), and “aspect ratio” between the c-axis parallel and perpendicular axes lengths. First, whole, unpolished synthetic grains were created with sizes (L_1 and L_2) including “Smallest” ($60 \mu\text{m}$), “Small” ($100 \mu\text{m}$), “Medium” ($150 \mu\text{m}$), or “Large” ($200 \mu\text{m}$), a range of aspect ratios where the first axis (W_1) was set to 0.3-1 times the size, and a range of width ratios where the second short axis (W_2) was set to 0.5 – 1 times W_1 . The range of c-axis parallel sizes was chosen to reflect sizes commonly seen in natural zircon. Aspect and width ratio ranges were chosen to reflect observed ranges of these ratios while also ensuring that grinding depth would always be greater than one alpha stopping distance. This was done to ensure no complications to interpreting F_T arising from incomplete removal of the alpha-ejection rim. Grains were created in this way for all common zircon idealized geometries: ellipsoid, cylinder, and tetragons with no, one, or two terminations. “Polished grains” were then created by assigning grinding depth as a fraction of the total width or length of the grain depending on whether grains were polished parallel or perpendicular to the c-axis, respectively. The range of grinding depths includes 0 (unpolished grains) and 0.25-0.75 of the total width or length.”

I have also added more description of the Ketcham et al. and Reiners et al. methods:

Line 61-63: “For grains polished parallel to the c-axis Reiners et al. (2007) provides a protocol for a limited number of cases: cylindrical and orthorhombic prisms ground and polished to a depth between one alpha-stopping distance and less than half of the original c-axis perpendicular thickness of the crystal.”

Line 201-206: “Although the Ketcham et al. protocol is not designed for polished grains, it might be assumed that the difference in final F_T value obtained by applying it might be negligible due to the application of the same polynomial coefficients in both methods. Here, the methods are compared to show that systematic biases are introduced when a whole-grain protocol is applied to polished grains that can result in limited utility of the dataset. This comparison was achieved by duplicating the synthetic dataset and setting grinding depth g equal to 0 for all synthetic grains so that the code treated them as unpolished for calculating V and SA_α , and F_T .”

Line 231-244: “The Reiners et al. (2007) protocol uses V and SA_α of grain fragments with the F_T formulas and polynomial coefficients of Farley (2002) but it applies only to cylindrical and non-terminated tetragonal grain geometries polished less than halfway through the original width of the crystal. For grains with maximum symmetry (Fig. 3c), the synthetic F_T results of the Reiners et al. protocol are almost identical to the new protocol, with all F_T values > 0.5 . In these cases, the calculation of SA_α and V are the same between the two methods and any discrepancy is the result of differences between the polynomial coefficients used. However, systematic offsets related to grain geometry appear when comparing F_T for cylindrical grains with minimal symmetry (Fig. 3d). For cylindrical grains, the Reiners et al. protocol results in higher F_T values than the new protocol reflecting that the Reiners et al. protocol assumes grains are true cylinders with symmetry about the c-axis. This results in underestimates of SA_α and V compared to the new protocol which treats cylinders as prisms with ellipsoidal pinacoid terminations. For tetragonal grains, F_T values calculated using the new protocol are larger than values calculated using the Reiners et al. protocol. Tetragonal SA_α and V are calculated using the same formulas regardless of protocol, so differences arise solely from

the difference in polynomial coefficients. Although there is not a significant difference in the number of grain fragments with $F_T > 0.5$ between the new and Reiners protocols, the addition of ellipsoid grains and the greater range of grinding depths covered under the new protocol makes it an improvement over the existing Reiners et. al. method.”

RC1: Line 189: Please clarify what you mean with ‘uncorrected method’?

AC: The use of “uncorrected method” in this context was meant to differentiate the method of Ketcham et al. (2011) for calculating volume, surface area, and F_T for whole grains from my protocol for calculating these values for polished grain fragments. As stated throughout the text, my protocol draws heavily on the approach and equations employed by Ketcham et al. but modifies them to reflect the volume and alpha-ejection surface area of polished grain fragments. However, based on this and other comments, this wording has only created confusion. The revised manuscript refers simply to the “Ketcham et al. protocol” in contrast to the “new protocol” presented in the manuscript.

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, F_T correction, and other derived values for polished zircon”... At the end of the day, the F_T correction is what most readers are interested in.

AC: I agree, thank you for the suggestion. The title has been revised to:

“Technical Note: Improved calculation of volume, F_T correction, and other derived data for polished zircon (U-Th)/Thermochronology”

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 further discussion of the differences between methods would strengthen the manuscript. Notably, the conditions under which the different protocols are designed to apply are very different. I agree that this is an important point that was missing from the manuscript, and it has now been added.

Line 61-63: “For grains polished parallel to the c-axis Reiners et al. (2007) provides a protocol for a limited number of cases: cylindrical and orthorhombic prisms ground and polished to a depth between one alpha-stopping distance and less than half of the original c-axis perpendicular thickness of the crystal.”

Line 201-206: “Although the Ketcham et al. protocol is not designed for polished grains, it might be assumed that the difference in final F_T value obtained by applying it might be negligible due to the application of the same polynomial coefficients in both methods. Here, the methods are compared to show that systematic biases are introduced when a whole-grain protocol is applied to polished grains that can result in limited utility of the dataset. This comparison was achieved by duplicating the synthetic dataset and setting grinding depth g equal to 0 for all synthetic grains so that the code treated them as unpolished for calculating V and SA_α , and F_T .”

Line 231-244: “The Reiners et al. (2007) protocol uses V and SA_α of grain fragments with the F_T formulas and polynomial coefficients of Farley (2002) but it applies only to cylindrical and non-terminated tetragonal grain geometries polished less than halfway through the original width of the crystal. For grains with maximum symmetry (Fig. 3c), the synthetic F_T results of the Reiners et al. protocol are almost identical to the new protocol, with all F_T values > 0.5 . In these cases, the calculation of SA_α and V are the same between the two methods and any discrepancy is the result of differences between the polynomial coefficients used. However, systematic offsets related to grain geometry appear when comparing F_T for cylindrical grains with minimal symmetry (Fig. 3d). For cylindrical grains, the Reiners et al. protocol results in higher F_T values than the new protocol reflecting that the Reiners et al. protocol assumes grains are true cylinders with symmetry about the c-axis. This results in underestimates of SA_α and V compared to the new protocol which treats cylinders as prisms with ellipsoidal pinacoid terminations. For tetragonal

grains, F_T values calculated using the new protocol are larger than values calculated using the Reiners et al. protocol. Tetragonal SA_α and V are calculated using the same formulas regardless of protocol, so differences arise solely from the difference in polynomial coefficients. Although there is not a significant difference in the number of grain fragments with $F_T > 0.5$ between the new and Reiners protocols, the addition of ellipsoid grains and the greater range of grinding depths covered under the new protocol makes it an improvement over the existing Reiners et. al. method.”

Regarding why the protocols differ, I have addressed this by adding protocol evaluation using a synthetic dataset that includes many more possible scenarios than the real dataset originally presented. This is now in the main text of the manuscript, while the real data example has been moved to a supplement. Grain size and grain symmetry are the dominant factors in how different the results of the different protocols are to each other. Large, symmetric grains give relatively similar results regardless of protocol, while smaller, less symmetric grains differ more significantly. This is shown and discussed in a completely new Section 3 and two figures (Lines 162-258; Fig. 2, 3).

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 F_T ?

AC: I agree showing any apparent trends in the difference between protocols would be useful. Rather than adding histograms, I have opted to for minimal figures but I have added discussion of when and why protocols are the same and different and annotations to Figure 3 to show how trends in the difference between protocols with increased grinding depth.

Line 206-215: “For the most symmetric grains (aspect and width ratios of 1, Fig. 3a), applying the whole-grain Ketcham et al. protocol results in F_T values that are generally lower than the new protocol. This is expected: the Ketcham et al. protocol calculates SA_α that is higher than the real polished SA_α in all cases, and in the case of ellipsoids calculates V that is significantly smaller than the real polished V . If the recommended 0.5 F_T cutoff for accepting (U-Th)/He analyses is applied (e.g., Flowers et al., 2022b) to the polished fragments, use of the Ketcham et al. protocol would result in rejection of more ellipsoid, cylindrical, and terminated tetragonal grains than the new protocol while more non-terminated tetragonal grains would be kept. This is because the only difference between the two protocols for non-terminated tetragonal grains is the inclusion of the polished face in SA_α . For grains with the least symmetry, both protocols result in the rejection of most grain fragments, but the Ketcham et al. protocol results in more total rejections due to its inaccurate estimates of V and SA_α .”

Line 233-243: “For grains with maximum symmetry (Fig. 3c), the synthetic F_T results of the Reiners et al. protocol are almost identical to the new protocol, with all F_T values > 0.5 . In these cases, the calculation of SA_α and V are the same between the two methods and any discrepancy is the result of differences between the polynomial coefficients used. However, systematic offsets related to grain geometry appear when comparing F_T for cylindrical grains with minimal symmetry (Fig. 3d). For cylindrical grains, the Reiners et al. protocol results in higher F_T values than the new protocol reflecting that the Reiners et al. protocol assumes grains are true cylinders with symmetry about the c-axis. This results in underestimates of SA_α and V compared to the new protocol which treats cylinders as prisms with ellipsoidal pinacoid terminations. For tetragonal grains, F_T values calculated using the new protocol are larger than values calculated using the Reiners et al. protocol. Tetragonal SA_α and V are calculated using the same formulas regardless of protocol, so differences arise solely from the difference in polynomial coefficients.”

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.

For example, the author states that “The Reiners et al. method of accounting for F_T 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 further discussion and justification of this method compared to others was necessary. I have addressed this with the use of the synthetic dataset to show the dominant factors that control differences between methods and how more accurately calculating V and SA_α through the added complication of geometry classification and measurements results in more usable grains and thus more data. I have also revised the text in the Introduction, Section 2, and Section 3 to be explicit about the fact that existing methods do not apply to many common scenarios.

Line 59-72: “Although this approach can be applied to any crystal geometry and plane of symmetry, the He and Reiners protocol is focused on cylindrical grains polished or broken perpendicular to the c-axis. For grains polished parallel to the c-axis Reiners et al. (2007) provides a protocol for a limited number of cases: cylindrical and orthorhombic prisms ground and polished to a depth between one alpha-stopping distance and less than half of the original c-axis perpendicular thickness of the crystal. In reality, zircon encompass a range of morphologies depending on lithology and geologic history which can be approximated as cylinders, ellipsoids, and orthorhombic prisms with or without pyramidal terminations (commonly referred to as “tetragonal” geometries even when a- and b-axis measurements are not equivalent). The grinding and polishing orientation of individual crystals can be parallel or perpendicular to the crystallographic c-axis, and because of the natural variation in crystal size, it is common for polishing to remove a variable amount of crystal when multiple crystals are mounted and prepared together (e.g., Fig 1a). Protocols to determine F_T corrections and other derived data for polished zircon based on geometry and volume must therefore encompass these different scenarios in order to maximize the number of grains that can be used for analysis in a given sample and grain mount. To address the lack of a comprehensive approach to volume-derived data for polished zircon, this contribution presents a protocol...”

Line 201-217: “Although the Ketcham et al. protocol is not designed for polished grains, it might be assumed that the difference in final F_T value obtained by applying it might be negligible due to the application of the same polynomial coefficients in both methods. Here, the methods are compared to show that systematic biases are introduced when a whole-grain protocol is applied to polished grains that can result in limited utility of the dataset. This comparison was achieved by duplicating the synthetic dataset and setting grinding depth g equal to 0 for all synthetic grains so that the code treated them as unpolished for calculating V and SA_α , and F_T . For the most symmetric grains (aspect and width ratios of 1, Fig. 3a), applying the whole-grain Ketcham et al. protocol results in F_T values that are generally lower than the new protocol. This is expected: the Ketcham et al. protocol calculates SA_α that is higher than the real polished SA_α in all cases, and in the case of ellipsoids calculates V that is significantly smaller than the real polished V . If the recommended 0.5 F_T cutoff for accepting (U-Th)/He analyses is applied (e.g., Flowers et al., 2022b) to the polished fragments, use of the Ketcham et al. protocol would result in rejection of more ellipsoid, cylindrical, and terminated tetragonal grains than the new protocol while more non-terminated tetragonal grains would be kept. This is because the only difference between the two protocols for non-terminated tetragonal grains is the inclusion of the polished face in SA_α . For grains with the least symmetry, both protocols result in the rejection of most grain fragments, but the Ketcham et al. protocol results in more total rejections due to its inaccurate estimates of V and SA_α . This is important for real datasets in which grain aspect and width ratios can be expected to vary widely and rarely match the maximum symmetry case. By taking grinding and polishing into account, the new protocol results in F_T values that reflect the true SA_α and V of the measured grain fragment and are more likely to meet the criteria for being accepted.”

Line 231-244: “The Reiners et al. (2007) protocol uses V and SA_α of grain fragments with the F_T formulas and polynomial coefficients of Farley (2002) but it applies only to cylindrical and non-terminated tetragonal grain geometries polished less than halfway through the original width of the crystal. For grains with maximum symmetry (Fig. 3c), the synthetic F_T results of the Reiners et al. protocol are almost identical to the new protocol, with all F_T values > 0.5 . In these cases, the calculation of SA_α and V are the same between the two methods and any discrepancy is the result of differences between the polynomial coefficients used. However, systematic offsets related to grain geometry appear when comparing F_T for cylindrical grains with minimal symmetry (Fig. 3d). For cylindrical grains, the Reiners et al. protocol results in higher F_T values than the new protocol reflecting that the Reiners et al. protocol assumes grains are true cylinders with symmetry about the c-axis. This results in underestimates of SA_α and V compared to the new protocol which treats cylinders as prisms with ellipsoidal pinacoid terminations. For tetragonal grains, F_T values calculated using the new protocol are larger than values calculated using the Reiners et al. protocol.

Tetragonal SA_α and V are calculated using the same formulas regardless of protocol, so differences arise solely from the difference in polynomial coefficients. Although there is not a significant difference in the number of grain fragments with $F_T > 0.5$ between the new and Reiners protocols, the addition of ellipsoid grains and the greater range of grinding depths covered under the new protocol makes it an improvement over the existing Reiners et. al. method.”

RC2: 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 F_T 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 Introduction and Section 2 have been revised to include description of the He and Reiners (2022) approach and shared aspects with the new protocol.

Line 56-61: “... the same symmetry logic can be applied to crystals broken perpendicular to an axis of symmetry when the true original axis length is unknown (He and Reiners, 2022). The broken interior face of the crystal is treated as a plane of symmetry such that the fragment has the same F_T as a whole grain with an axis length double the axis length of the fragment. V and SA_α of the fragment can be calculated by dividing the V and SA_α of the reconstructed whole grain in half. Although this approach can be applied to any crystal geometry and plane of symmetry, the He and Reiners protocol is focused on cylindrical grains polished or broken perpendicular to the c -axis.”

Line 92-96: “In most cases, calculating these values is accomplished by adopting the same approach as He and Reiners (2022) in which the polished grain is treated as a crystal broken along a plane of symmetry such that V and SA_α of the polished fragment are half of a whole “assumed grain” created by reflecting the existing fragment across the plane of polishing (Fig. 1c). F_T of the fragment is thus equal to F_T of the assumed grain.”

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 F_T corrections assumes that the polynomial function relating SA/V to F_T 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 - F_T functions.

AC: I agree that this is worth discussing. I based my protocol on F_T equations from Ketcham et al. (2011) rather than Farley (2002) precisely because the Ketcham et al. equations are tailored to specific geometries. I have added a paragraph to Section 2 discussing in general how F_T is calculated and polynomial coefficients.

Line 123 - 140: “ F_T depends not just on volume, but also on SA_α dependence which is represented here using the term R_{SV} , or volume-to-surface-area equivalent spherical radius, calculated using Eq. (2) as in Ketcham et al. (2011).

$$R_{SV} = \frac{3V}{SA_\alpha} \quad (2)$$

R_{SV} serves the same function as the β term introduced by Farley (2002) to relate grain measurements to F_T via a polynomial function with the general form of Eq. (3).

$$F_T = 1 + a_1\beta + a_2\beta^2 + a_3\beta^3 + \dots \quad (3)$$

Polynomial coefficients a_1 , a_2 , and a_3 , etc. are determined via series of Monte Carlo simulations of variable grains and fitting the results (e.g., Hourigan et al., 2005; Ketcham et al., 2011) and depend on alpha-stopping distance and grain geometry. For the new protocol, the F_T equations and coefficients of Ketcham et al. (2011) are adopted as the basis for calculating F_T (Appendix A) because they are fit to the full range of grain geometries commonly seen in natural zircon. For grains that begin whole as ellipsoids, cylinders, or tetragons without terminations, grinding and polishing results in remaining grain fragments with morphologies that are still well-described by the original geometries and F_T equations tailored to those geometries, such that minimal uncertainty is introduced by applying the geometry-specific coefficients of Ketcham et al. to these polished grains. The whole-grain coefficients are likely less applicable to grain geometries that change more significantly with grinding and polishing, namely tetragonal geometries with one or two terminations, and the new protocol should be applied with caution to these geometries. However, even with this

limitation, the new protocol improves on existing protocols for polished grain F_T values through the addition of ellipsoid geometries and a range of polishing depth beyond half of the original grain width.”

RC2: It’s not clear from Fig. 1 what the different labels (e.g. w_1 w_p) are referring to in many of the diagrams.

AC: Thank you for the feedback that this is unclear. W_1 , W_2 , L_1 , and L_2 are the measurements made of the grain while a , b , c , and h refer to the axes, semi-axes, and 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 W_1 , L_1 and W_2 , L_2 measurements are made by rotating the grains 90° such that these measurements can also define a rectangular prism that surrounds the grain, shown in revised Figure 1. To help clarify these relationships I have added text to Section 2

Line 83-85: “Like standard approaches for calculating whole-grain V (e.g., Zeigler et al., 2024), two orthogonal sets of length and width measurements (L_1 , W_1 and L_2 , W_2), are made by rotating the grain fragment (Fig. 1b).”

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 Line 89-90. To further distinguish alpha-ejection surface area from total surface area I have adopted your suggestion of using an alpha subscript throughout the text. I have also added explanation of how R_{SV} relates to β and the relationship of both to F_T .

Line 123 - 129: “ F_T depends not just on volume, but also on SA_α dependence which is represented here using the term R_{SV} , or volume-to-surface-area equivalent spherical radius, calculated using Eq. (2) as in Ketcham et al. (2011).

$$R_{SV} = \frac{3V}{SA_\alpha} \quad (2)$$

R_{SV} serves the same function as the β term introduced by Farley (2002) to relate grain measurements to F_T via a polynomial function with the general form of Eq. (3).

$$F_T = 1 + a_1\beta + a_2\beta^2 + a_3\beta^3 + \dots \quad (3)$$

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: The explanation of how grains are measured and classified by geometry has been expanded in Section 2.

Lines 79-87: “The protocol presented here adapts existing approaches for determining whole-grain V , SA_α , and F_T for ground and polished grain fragments. First, the polished grains are removed from the mounting medium and inspected and measured using a binocular microscope with digital camera and microscope imaging software. Grains are classified as ellipsoidal, cylindrical, or “tetragonal” geometries, which can include two, one, or no pyramidal terminations. In order to be classified as cylindrical or tetragonal, the unpolished part of the grain must include visible crystal faces that are unrelated to the polished face. For cylinders, these faces are only perpendicular to the long axis while for tetragonal grains, some must be parallel to the long axis (Fig 1). If there are no observed crystal faces, the grain is classified as an ellipsoid. Like standard approaches for calculating whole-grain V (e.g., Zeigler et al., 2024), two orthogonal sets of length and width measurements (L_1 , W_1 and L_2 , W_2), are made by rotating the grain fragment (Fig. 1b).”

The description and discussion of the real dataset has been moved to a Supplement, and I have updated it with inclusion of grain size distribution and other descriptors.

Lines S21-S31: “The real dataset ($n = 70$, Table S2) includes a much more limited sampling of original grain geometries, grain sizes, aspect ratios, and width ratios than the synthetic dataset. Geometries include ellipsoids ($n =$

58), cylinders ($n = 8$), non-terminated tetragons ($n = 3$) and tetragons with one termination ($n = 1$). The high number of ellipsoidal grains is unsurprising given grain abrasion that occurs during sediment transport. Size (c-axis parallel length) ranges from 102 to 361.1 μm with a median size of 199.3. Aspect ratio (the ratio between the c-axis parallel length and larger perpendicular axis) ranges from 0.3209 to 2.5222 with a median of 1.0669. Width ratio (the ratio between the two c-axis perpendicular axes) ranges from 0.3303 to 0.9929 with a median of 0.6528. The aspect ratios and width ratios present in the real dataset are similar to the ranges tested with the synthetic dataset. However, the real dataset only includes zircon with c-axis parallel size in the higher end of the range, or higher than sizes tested with the synthetic dataset. Grinding depth was significantly, calculated using measurements of mounted glass beads as in Section 2 of the main text, was significantly higher than the zircon average alpha stopping distance in all cases (Table S2).”

All grain measurements L_1 , L_2 , W_1 , W_2 , and R_{SV} and R_{FT} proxies for grain size for each individual grain are included in Table S2.