NOTES ON STATISTICAL AGE DISPERSION IN FISSION-TRACK DATASETS: THE CHI-SQUARE TEST, ANNEALING VARIABILITY, AND ANALYTICAL CONSIDERATIONS

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The manner in which we apply statistical analysis is founded on an idealized concept of how fission tracks are generated and measured, which may be more complicated in practice when there are departures from ideal circumstances. The fission track (FT) method is a low precision technique, and we beat this shortcoming with numbers, that is to say, by repeating many low precision individual analyses to provide a better estimate of some 'true' age or to make inferences about the overall age population. The chi-square (χ^2) test is a simple diagnostic used to assess whether single-grain age estimates are statistically homogenous and consistent with a common true age [1]. Significance of the test is assessed by calculating the *p*-value, which is the probability that a value drawn from the χ^2 (n-1) distribution exceeds the χ^2 statistic [1]. A small *p*-value indicates that the data are inconsistent with a common ρ_s/ρ_i ratio for the external detector method, EDM, or a common value of $N_s/(^{238}U/^{43}Ca)$ for the apatite LA-ICP-MS ζ-method. The convention being that a *p*-value < 0.05 offers sufficient evidence against the null hypothesis (of a common true age) and a *p*-value < 0.01 is strong evidence against the null hypothesis [1]. Typically, a χ^2 value of < 0.05 is considered to indicate that the single-grain ages are unlikely to be drawn from a single Poissonian distribution with a discrete mean value and may represent multiple age populations [1–3]. However, a large *p*-value only means there is a lack of evidence against the null hypothesis—it does not lend support for an alternative hypothesis [1].

The χ^2 test applied to FT data is not a data quality filter. A χ^2 pass or failure does not equate to 'good' or 'bad' fission track data, respectively. A sample should still undergo evaluation if it passes the χ^2 test, and if a sample fails, an attempt should be made to understand why it failed. Even though the χ^2 statistic is designed to test the underlying assumption of a single, underlying age for a sample, a problem encountered in many published fission-track studies is that the results of the χ^2 test are noted when a sample passes, but are ignored or downplayed if the sample fails—leading to a tendency to incorrectly judge the quality of FT data based on the χ^2 test. This is likely due to the fact that without more information, we do not necessarily know how to explain a χ^2 failure. For example, it has been acknowledged for decades that chemical composition is a control on fission-track thermal annealing and consequently FT ages [e.g., 4–8], however many studies lack proper quantification of mineral composition to evaluate potential cause(s) of high age dispersion and χ^2 failure. The amount of thermal annealing, and therefore FT shortening, experienced by a sample may differ between grains due to variable chemical composition [2, 5–9]. In this case, a *distribution* of FT single-grain ages should exist, rather than a single common value [1, 3]. This point is critical—if a crystalline basement or detrital fission-track sample is characterized by variable intragrain chemical composition (or additionally, variable provenance for detrital samples) and has experienced thermal annealing—then a χ^2 failure should be expected. This sample would be considered multikinetic and if the relationship between mineral chemical composition and discrete age populations can be characterized, then each kinetic population within a sample will be sensitive to a specific temperature range (i.e. variable thermal annealing kinetics), broadening the overall sensitivity of the sample [10–12]. This essentially means that multiple thermochronometers are contained within a single sample—characterized by kinetic age populations with distinctive annealing behavior. Multikinetic behavior is useful because it allows the user to 'do more with less,' in that we can constrain more thermal information with a single sample and yield improved time-temperature resolution for thermal history analysis, which is often the goal of nearly all FT studies.

Fission track analysis is a geochronological method that is highly dependent on choices made by an analyst. Therefore, evaluating, monitoring for, and mitigating fission-track analyst bias should not be marginalized by users of fission-track data [13, 14]. Complex Earth system interactions often produce complex datasets that are difficult to interpret or understand if we do not have all the necessary information at our disposal. Consequently, fission track datasets that are 'too good' with perfect 100% χ^2 passes should not be expected in every case and require scrutiny like any other heteroscedastic dataset. Imagine a hypothetical scenario where an old crystalline basement sample yields Precambrian apatite FT ages. Most of the time we would assume a priori that this sample *should* yield a single age population and pass the χ^2 test, since all apatite grains are derived from the same rock. The analyst may struggle to find suitable grains for measurement due to high track density in many grains on the mount and select those considered easier to measure, unconsciously biasing towards younger ages. The analyst could also only count some, but not all, of the tracks in the counting area, which would yield low N_s totals and magnify the individual age errors. Ultimately, the central age would be representative for the sample, and we would have a χ^2 pass. The sole source apatite assumption and omission of apatite elemental data would implicitly validate our glowing statistics—but this may not be valid.

"Mistakes often come from assuming something is true just because there is little or no evidence against it." —R. Galbraith, *Statistics for Fission Track Analysis*, p. 190.

In addition to analyst bias, analytical canon has been to measure (up to) 20 age grains and 100 track lengths per sample. The χ^2 test is sensitive to sample size. The power of χ^2 increases when sample size is large enough and the absolute differences between individual ages become a progressively smaller proportion of the expected or 'true' value [15]. This means that any small deviations from an assumed 'true' age model in the dataset may appear statistically significant and provide support for the addition of mixture model age peaks [15]. Basically, the alternative to the null hypothesis is a very general one when n is large. Therefore, the higher the number of grains analyzed for an FT dataset, there is greater potential to fail the χ^2 test due to sample size [2], which is even more likely if single-grain ages are high precision.

There are other factors that are important when assessing and dealing with fission track age dispersion that require attention when interpreting a dataset. Some of the factors that play a role in statistical age dispersion include: (*i*) the total number of grains analyzed, (*ii*) the precision of individual fission track grain ages within a population, and (*iii*) the number of spontaneous tracks (N_s) counted by the analyst. Uranium concentration and N_s are the main contributors to the analytical uncertainty during fission track data collection [16, 17]. There is some concern that the standard error of LA-ICP-MS ages may be underestimated, causing age over-dispersion, and that the lack of a 'matched pairs' design (as with the EDM), may produce inaccurate ages due to difficulty in accounting for U heterogeneity [16]. This is more of an issue for very young or U-poor apatite grains, but ways to alleviate this are to only count tracks in the laser ablation spot area or to carry out multiple U spot analyses on a grain [16].

Nevertheless, a closer examination of LA-ICP-MS U error propagation and accounting may be warranted.

Young or U-poor samples typically have low N_s and larger associated errors, whereas old or U-rich samples have high N_s and higher precision ages. Generally, if a population of grain ages is characterized by low precision, then there is a χ^2 pass (p-value > 0.05) and low overall age dispersion would be expected, whereas if a dataset contains highly precise ages, then a χ^2 failure would be expected [1, 2]. The order-of-magnitude better age precision obtained by the LA-ICP-MS fission track technique (partly due to direct and more precise measurement of U compared to the EDM) will often produce χ^2 failures that are difficult to interpret without additional information such as mineral composition and complicates parsing of kinetic populations that align with radial plot mixture model predictions. In short, the results of LA-ICP-MS mixture modeling are often difficult to interpret (especially crystalline samples) and may fail simply because of high age precision (e.g., underestimated single-grain age uncertainties).

The differences in precision between the EDM and LA-ICP-MS methods is at least partially related to N_s counts and the number of grains analyzed. For instance, we have unpublished Precambrian basement samples that have LA-ICP-MS AFT single-grain age uncertainties of ~8–11% (1σ) on average, whereas EDM age uncertainties for the same samples are ~20–26% (1σ) on average. This difference in age precision alone can account for the majority of LA-ICP-MS AFT χ^2 test failures. In our experience, most Precambrian samples dated by LA-ICP-MS mostly fall into the range of ~5–10% uncertainty for single-grain ages [2]. This greater precision is even more influential for old samples with high spontaneous track densities (and/or high U content) since the number of spontaneous tracks account for most of the AFT analytical uncertainty [13, 15, 16]. We momentarily ignore the instrumental/analytical error contribution to the total ICPMS AFT age uncertainty. The precision related to N_s is more apparent when examining isolated uncertainties for track counts between hypothetical apatite grains with $N_s = 1$, where $\sqrt{1}/1 = 100\%$ error; $N_s = 100$, where $\sqrt{100}/100 = 10\%$ error; and $N_s = 400$, where $\sqrt{400}/400 = 5\%$ error. Many of our old samples have N_s counts much greater than 100, and often approach > 150 to 400 tracks. This suggests to us that single-grain N_s counts ≤ 100 are perhaps unconsciously ideal from an analytical perspective to maintain adequate count and sample precision, and that there may be both explicit biases (i.e., to obtain χ^2 passes) and implicit biases (i.e., analyst confidence/experience) against routinely counting high N_s grains.

An exaggerated example to illustrate the effect of age errors is shown by FIGURE 1 using a radial plot [18, 19] to graphically display single-grain ages and their precisions for two synthetic samples of 20 grains each with randomly generated ages between 50 to 100 Ma. We hold the grain ages fixed for both samples and only change the individual age errors at random. The first sample is precise (i.e., more ages further from the origin on the radial plot; FIGURE 1A), with individual grain-age errors varying between ~5–15%, while the second sample is low precision (FIGURE 1B) with age errors between ~12–85%. The errors on individual ages influence the sample χ^2 probability (0.0 vs. 0.98), age dispersion (20% vs. 0%), and the central age of the sample (~75 Ma vs. ~83 Ma), as well as modify the mixture model ages and the number of peaks identified during deconvolution [19–21]. If we were to assume that FIGURE 1B was a realistic case, then the mixture modeling in FIGURE 1A would be geologically meaningless. For the LA-ICP-MS method, χ^2 test failure and spurious mixture model age peaks should be expected if there are more counted grains (i.e., greater n) with high N_s densities (lacking a correlation between ages and apatite composition). The reader is referred to cited references 1, 2, 13, 15, and 16 for further discussion of these topics.

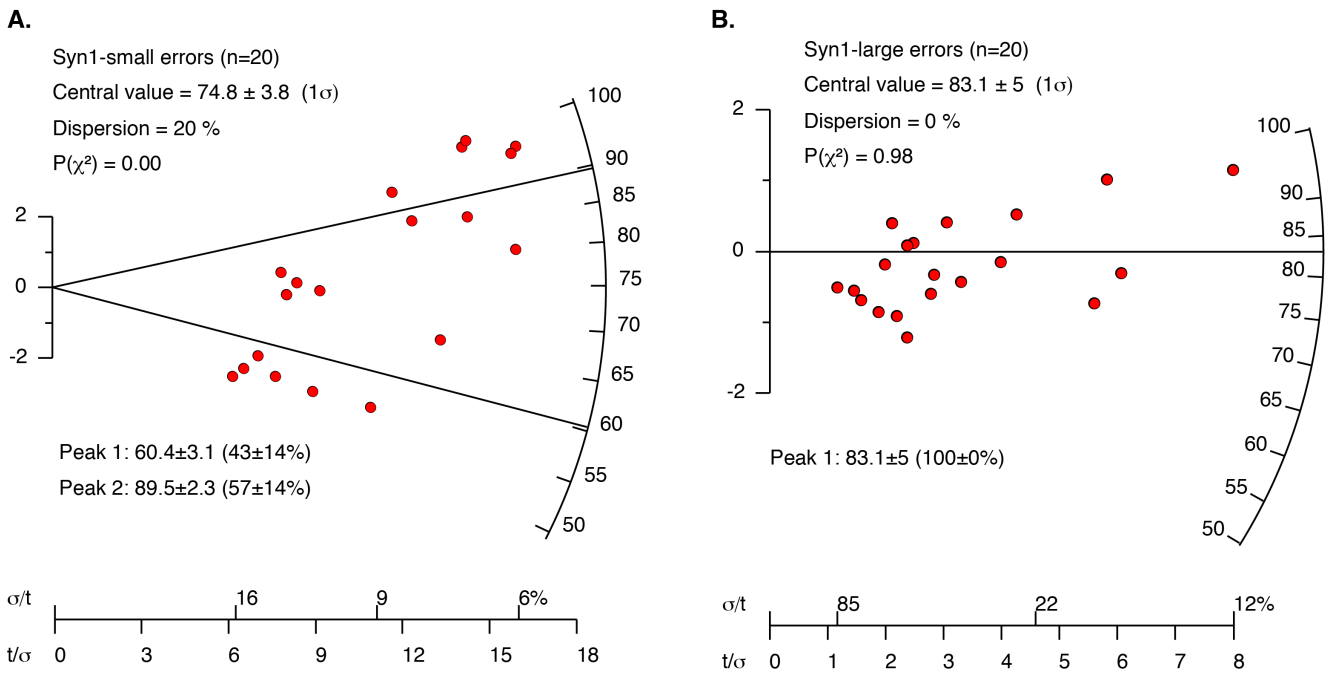

FIGURE 1. *(A) Radial plot for synthetic sample with precise single-grain ages. (B) Radial plot for same synthetic sample as (A) with lower precision single-grain ages. Grain ages were held fixed whereas errors were randomly assigned for both samples. Plots created with DensityPlotter v. 8.4 [ref. 19].*

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