Calculating isotope anomalies: a Bayesian approach

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Isotopic anomalies - the deviation of an isotopic ratio from a mass fractionation law (MFL) - allow us to study a wide variety of processes ranging from nucleosynthesis to radiometric dating. As such, knowledge of the MFL appropriate for a given isotopic system is critical for accurate calculations of isotopic anomalies.

In practice, the MFL is often assumed based either on community practice or computational convenience, rather than on physical reasoning. For example, evaporation of Ca-Al-rich inclusions (CAIs) fractionates Mg isotopes along a MFL that differs from the widely used exponential law [1].

Some studies [*e.g.*, 2] recognize that the choice of MFL can affect the conclusions drawn from isotopic data. For example, an incorrectly chosen MFL can affect the goodness of fit of isochrons. However calculating the MFL that optimizes the goodness of fit to an isochron [2] is without physical justification. In fact, such an approach is detrimental as it leads to claims of spuriously high precision.

We address these limitations (e.g., having to assume a single MFL) by proposing a new calculation method, based on Bayesian statistics, that allows us to explicitly incorporate uncertainties on the MFL as well as the timing of when the fractionation occurs relative to incorporation of the anomaly (e.g., before or after ingrowth from radioactive decay) into the final isotopic anomaly reported. We apply our new procedure to published Mg isotope data in CAIs and angrites in order to assess the effects on the short-lived ²⁶Al chronology. Our calculations show that the initial δ^{26} Mg of CAIs cannot be ascertained with precisions better than ~0.1‰ (1σ) . This arises from the fact that CAIs have fractionated Mg, though usually by a constant amount, and therefore the intercept (initial δ^{26} Mg) is dependent on the chosen MFL. By incorporating the uncertainty on the MFL into our calculations, we can provide accurate uncertainties on the initial δ^{26} Mg. Progress in constraining the ²⁶Al decay system can be made by determining appropriate values for the mass fractionation law used to correct Mg isotope data in a variety of settings. [1] Davis et al. (2015) GCA 158, 245-261. [2] Wasserburg et al. (2012) MAPS 47, 1980-1997.