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A Log-Ratio-Based Algorithm for Petrologic Mass-Balance Problems and Uncertainty Assessment

MIKE KRAWCZYNSKI[1], KELSEY PRISSEL[2] AND JEAN-ARTHUR OLIVE[3]

[1]Washington University in St. Louis
[2]Purdue University
[3]Laboratoire de Géologie, CNRS - École normale supérieure - PSL University

Presenting Author: mikekraw@wustl.edu

"The principle of mass balance is simply: some of it, plus the rest of it, equals all of it."—Stormer, Jr. and Nicholls (1978, https://doi.org/10.1016/0098-3004(78)90083-3). In the study of igneous and metamorphic rocks, mineral abundances are used to classify rock types, characterize volcanic processes, and define chemical reactions. Common approaches for calculating phase abundances, such as multiple linear regression, suffer from mathematical artifacts that can lead to inaccurate assumptions (e.g., Chayes, 1960, https://doi.org/10.1029/jz065i012p04185; Miesch, 1969, https://doi.org/10.1007/978-1- 4615-8633-3_10).

Here we present a new algorithm for mass-balance calculations in petrology and geochemistry based on the log-ratio approach championed initially by John Aitchison (e.g., Aitchison, 1982, https://doi. org/10.1111/j.2517-6161.1982.tb01195.x; Aitchison, 1984, https://doi.org/10.1007/bf01029316) along with the underlying principles, mathematical frameworks, and data requirements. Log-ratio Inversion of Mixed End-members (LIME) is written in MATLAB and calculates phase proportions in an experiment or rock given a bulk composition, the composition of each phase, and the associated compositional uncertainties. An important advantage of LIME is that performing the mass-balance calculation in inverse log-ratio space constrains phase proportions to be between 0 and 100 wt.%. Further, the resulting LIME posterior distribution of plausible phase proportions provides realistic estimates of uncertainty regardless of data distribution. These two characteristics of LIME improve upon standard multiple linear regression techniques, which may yield negative values for phase proportions if non-constrained or report oversimplified symmetric errors. Importantly, this enables the users to propagate true uncertainty in phase proportions into subsequent calculations or regressions.

Primary applications of LIME include estimating phase abundances, calculating melting and metamorphic reaction stoichiometries, and checking for open system behavior in phase equilibria experiments. The technique presented here covers whole-rock analysis, mineralogy, and phase abundance, but could be extended to isotopic tracers, trace element modeling, and regolith component un-mixing. We highlight the importance of uncertainty estimations for phase abundances to the fields of petrology and geochemistry by comparing our results from LIME to previously published mass-balance calculations. Furthermore, we present case studies that demonstrate the role of mass-balance calculations in determining magma crystallinity and defining melting reactions.