Closure in compositional data analysis: is it always such a hazard?

CLIFFORD R. STANLEY

Department of Earth and Environmental Science, Acadia University, Wolfville, Nova Scotia B4P 2R6, Canada <cliff.stanley@acadiau.ca>

"Closure" is the mathematical constraint that component concentrations in a given system sum to 100%. Thanks to Felix Chayes, geoscientists have known for more than six decades that closure adds variation to compositional datasets and thus obscures variations caused by material transfer processes. In the late 1960s, Tom Pearce and others developed graphical, molar element ratio data analysis methods that avoid closure, thereby allowing recognition/ quantification of material transfer processes. More recently, John Aitchison and others developed alternative log-ratio methods that avoid closure in the statistical realm. Unfortunately, the passion of these log-ratio enthusiasts has given many geoscientists the impression that log-ratio methods are the ONLY way of circumventing closure, and thus that these methods MUST be used in any form of compositional data analysis in order to reach valid conclusions. This presentation disproves these misconceptions, illustrating that not only can compositional data be evaluated properly using techniques other than log-ratios, but that many geochemical systems contain elements that are not impacted significantly by closure at all, and thus need not be evaluated by any closure-avoiding data evaluation procedures.

An equation derived from the definition of a concentration allows one to assess the relative magnitudes of closure- and material transfer-induced relative variation. Functional analysis of this equation reveals that closure does not mask material transfer when: (i) the system size doesn't change during material transfer, (ii) the concentration of components undergoing material transfer are small, and (iii) the relative amount of material transfer of a component is large relative to the change in system size. Thus, this equation confirms what geoscientists have known intuitively since the dawn of geochemistry, that trace element concentrations generally do not suffer from closure, but major oxide concentrations commonly do, a feature that explains why miners have successfully extracted low concentration ores without the use of closure-avoiding data analysis methods for over a century.

To illustrate the above, two datasets are evaluated, one of feldspar compositions from a porphyry Cu deposit in Chile, and one of turbidite compositions from New Zealand. These evaluations demonstrate that the automatic use of closure-avoiding procedures in geochemical data analysis may be unnecessary, as some components, and even some geological systems, do not suffer from closure. Lastly, I illustrate strategies that allow the geoscientist to recognize, using conserved elements, which components of a system are affected by closure, and which are not, affording them the opportunity to take appropriate action to avoid closure only where necessary.

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