

Merging key concepts in the chemistry of natural waters with compositional data analysis

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Abstract

In the 12 years since the publication of “New perspectives on water chemistry and compositional data analysis” by Buccianti and Pawlowsky-Glahn (2005), substantial efforts have been made in understanding how to apply compositional data analysis (CoDa) in the interpretation of water quality data. Moreover, there is a better understanding of how to tie concepts (such as stoichiometry and chemical equilibrium) to log-ratio approaches. This paper intends to provide a broad overview and summary of the connections between the chemistry of natural waters and CoDa as well as a tool set of applied techniques, broken up into 4 themes.

The first theme will propose solutions to working with important but challenging water quality constituents and parameters in CoDa, namely water concentration (e.g., mg/L or mol/L), total dissolved solids, alkalinity, and isotopes (both stable and radiogenic). The second theme of this paper will cover similarities in concepts between CoDa and water chemistry as a means to assist in creation of log-ratios. In particular, chemical equilibrium and the Law of Mass Action will be covered as well as the idea of geochemical divides (Hardie and Eugster, 1970), an idea with important implications in the chemical evolution of brines and saline waters. With this knowledge, the paper will move onto CoDa-based graphical methods and their applications. Examples to be covered include log-ratio versions of scatterplots, Stiff diagrams, Durov plots, brine differentiation plots, and sodium-chloride-bromide based diagrams. In the final theme, CoDa-based methods to examine baseline or ambient water quality conditions will be examined and discussed. Our intention is that this work can be used to quickly bring an interested scientist up to speed with current knowledge and ideas and increase the application of CoDa methods in routine interpretation of water chemistry data.

References

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