

Chemical weathering from the CoDA (Compositional Data Analysis) point of view: new insights for the Alpine rivers geochemistry

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The aim of this contribution is to explore the relationship among weathering reactions, the sample space of compositional data and fractals by means of distributional analysis. Weathering reactions represent the transfer of heat and entropy to the environment in geochemical cycles. Chemical weathering is a key process for understanding the global cycle of elements, both on long and short-terms and chemical weathering rates are complex functions of many factors including dissolution kinetics of minerals, mechanical erosion, lithology. Compositional data express the relative (proportional) abundance of chemical elements/species in a given total (i.e. volume or weight) so that compositions pertaining to the peculiar geometry of the simplex sample space. Fractals are temporal or spatial objects with self-similarity and scale invariance, so that internal structures repeat themselves over multiple levels of magnification or scales of measurement.

Gibbs's free energy and the application of the Law Mass Action can be used to model weathering reactions, under the hypothesis of chemical equilibrium. Compositional data are obtained in the analytical phase after the determination of the concentrations of chemicals in sampled solid, liquid or gaseous materials. Fractals can be measured by using their fractal dimensions.

The presence of fractal structures can be observed when the frequency distribution of isometric log-ratio coordinates is investigated, showing the logarithm of the cumulative number of samples exceeding a certain coordinate value plotted against the coordinate value itself. Isometric log-ratio coordinates (or balances) can be constructed by using the sequential binary partition (SBP) method. The balances can be identified to maintain, as far as possible, the similarity with a corresponding weathering reaction (Buccianti & Zuo, 2016). As an alternative, balances can be derived after the multivariate investigation of the variance-covariance structure of the compositional matrix. In both cases the idea is to probe the behaviour of geochemical processes to be analysed in time or space. An application example is presented for the chemistry of the surficial waters of the Alpine region (Donnini et al., 2016). The emergence of fractal structures indicates the presence of dissipative systems, which require complexity, large numbers of inter-connected elements and stochasticity requiring caution in the use of classical spatial methods to represent geochemical phenomena.

Buccianti A. & Zuo R., 2016. Weathering reactions and isometric log-ratio coordinates: Do they speak to each other? Applied Geochemistry, 75, 189-199.

Donnini M., Frondini F., Probst J.L., Probst A., Cardellini C., Marchesini I., Guzzetti F., 2016. Chemical weathering and consumption of atmospheric carbon dioxide in

the Alpine region. Global and Planetary Change, 136 (2016) 65–81.