Redundant data in geochemical calculations: Helpful or not?

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Geochemical speciation problems require the solution of non-linear systems by means of numerical methods that can be computationally demanding and sometimes can even fail to reach convergence. The performances of those numerical methods have been therefore studied in the last decades in order to increase their robustness and to find the most suitable ones for different types of systems and constraints [1, 2].

Often the amount of information available about a geochemical system can be redundant, that is, exceed the requested minimum so that a least square fitting may be necessary [3]. In those cases, models can account for data uncertainty. The effect of error in data has been studied for specific problems such as solubility equilibrium or mixing fraction calculations [4, 5].

However, little attention has been paid to the contribution that redundant data might have in the characterization of geochemical systems and in particular which types of systems are most likely to take advantage of additional data.

We present an algorithm able to handle redundant uncertain constraints and the systems that have been analyzed in order to understand the importance of considering different types of extra data in equilibrium calculations.

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Continuous soil CO_2 flux measurements in a fumarole field of Mt Etna

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We present data from seven months of continuous measurements in the summit area of the Mt Etna volcano. The monitoring began in September 2012 and continued without any maintenance until the present (April 2013). The monitoring site is placed at “Belvedere” on the southeastern flank of the volcano, about 1.5 km away from the New Southeast Crater (NSEC) at altitude of about 2700 m a.s.l. This site is characterized by a low-temperature fumarole field. Performing soil CO2 flux measurements in such a hostile environment, particularly during the winter, is extremely challenging, and we took advantage of an innovative device named CADEMASO [1]. This device determines soil CO_2 flux by measuring the pressure transient in a closed polymeric tube inserted into the soil. The station recorded hourly soil CO_2 flux and soil temperature. The data set revealed two distinct periods with different characteristics. During the first period, which lasted until the second decade of November, the soil temperature was almost constant around 80°C with small fluctuations, whereas the soil CO_2 flux displayed wide oscillations. During the second period, the soil temperature values displayed sharply and long lasting increments, as high as the measurement limit (225°C).As regards the soil CO_2 flux, an overall decrement of the values was observed and several clearly defined peaks were recorded. The beginning of the last period coincides with the first signs of a new reactivation of the activity of the NCSE, after a period of rest of about seven months.

[1] De Gregorio *et al.*., (2013) Chem. Geol. 341, 102–109

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