

## Investigation of reactive transport with closed-flow column experiments and parallel factor analysis (PARAFAC) of fluorescence data

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The study of biogeochemical interfaces is crucial to understand soil functioning [1]. The sorption of solutes and colloids to these interfaces results in the phenomenon of retardation. Besides the interactions at the sorbent-solution-interface, the sorption rate depends also on the spatial structure of the pore network (size distribution, connectivity, topology). Column experiments allow for the consideration of the structure and thus for a quantification of possible rate limitations. We focus on column experiments run in closed-flow mode. There, a typical oscillation in the “breakthrough” of solute concentration, which conveys additional information about the flow regime (dispersivity, water content, immobile water) as well as the effective interaction kinetics, can be observed. Another major feature of the closed flow design is the conservation of tracer mass inside the column setup. Therefore, the investigation of sorption characteristics can be simplified by using mass balances.

Our objective was to study the interaction between different solutes (conservative tracers, e.g., NaCl and reactive tracers, e.g., acetate, oxalate and vanillic acid) and artificial porous media (composed of quartz, illite, goethite and charcoal in a well defined grain size distribution). The reactive tracers were chosen to probe specific reactive surfaces, which allowed for a consideration of involved sorption mechanisms and an estimation of sorbent surface coverage. The concentration-time profile of solutes was measured with non-consuming techniques (fluorescence spectroscopy or electrical conductivity measurements). PARAFAC analysis of fluorescence data was used for the quantification of aromatic compounds in complex background solutions. Since the reconstructed sorption characteristics are influenced by physical and chemical non-equilibrium and possible sorption sites were unavailable due to aggregate formation and immobile regions in the porous medium, we were able to estimate the amount of void volume and the availability of sorption sites of goethite.

[1] Totsche, Rennert, Gerzabek, Kögel-Knabner, Smalla, Spiteller & Vogel (2010), *J. Plant Nutr. Soil Sc.* **173**, 88-99.

## Hydrogeochemical modeling and noble gas analysis of spring waters from Poços de Caldas, MG-Brazil

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Thermal and non-thermal spring water samples from the city of Poços de Caldas were analysed with respect to their chemical composition and dissolved noble gas contents. The objective is a better understanding of the hydrogeochemical evolution, maximum reservoir temperature, groundwater age and possible heat sources of the low-enthalpy thermal system.

The genesis of the thermal alkaline waters (Na-K-(H)CO<sub>3</sub>-SO<sub>4</sub>-F-type) could be approached by an inverse model of water-rock interactions with PhreeqC. The model favours four main processes to take place in thermal water formation: (I) pyrite oxidation; (II) CaF<sub>2</sub> or NaF dissolution; (III) calcite precipitation; (IV) Na-K-alumosilicate weathering; (V) equilibrium at depth of Na and K with Na-K-alumosilicates (e.g. orthoclase and nepheline). Thoroughly chosen chemical Geothermometers, calculated with the computer program SolGeo [1], indicate maximum equilibrium reservoir temperatures of 105-130°C, which offer estimates on the circulation depth of 2.6-3.3 km.

Dissolved noble gas contents and their isotopic ratios in the water samples generally support previous assumptions [e.g. 2] of (i) different aquifer sources for the springs; (ii) the occurrence of mixing of thermal and non thermal water during ascent; and (iii) relatively long residence times of the circulating meteoric water in the geothermal system. Further noble gas data examination could lead to obtain age constraints derived by <sup>4</sup>He accumulation and more information about the heat source of the geothermal system.

[1] Verma, S. P., Pandarinath, K., & Santoyo, E. (2008). SolGeo: A new computer program for solute geothermometers and its application to Mexican geothermal fields. *Geothermics* **37**, p. 597-621. [2] Bonotto, D. M. (2005). The U-isotopes modelling in aquifers from Poços de Caldas plateau, Brazil. *Environmental Geology* **48**, p. 507-523.