Application of Hydrogeochemical Modeling Tools (PHREEQC/PHT3D) for Study of an Environmental Remediation Site

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Background/Objectives. In an industrial site located in Brazil, environmental investigations carried out in 15 km^2 pointed out the presence of barium in the groundwater with concentrations above the reference standards recommended by local environmental authorities, in two different centers of mass. Therefore, the plant at stake sized and implemented a remediation system based on injection and pumping processes, with mean flow rates around 250 m^3/h and 450 m^3/h, respectively. Nevertheless, given that the study area is formed by an anomalous geological context, such anomalies are expected to reverberate in the geochemical signature of groundwater, therefore, it may naturally show concentrations of some chemical elements above the reference standards established, including barium. This study aimed at understanding the evolution of the hydrogeochemical context of the groundwater of this area through application of mathematical modeling codes for assessment of two main points: (i) current hydrogeochemical equilibrium of the reactions of precipitation and dissolution of the minerals (Saturation Index – SI); (ii) three-dimensional evolution of multiparameter reactive transport (24 parameters) of the elements found in dissolved phase. In order to do so, the current occurrences of the elements in dissolved phase and their potential sources, natural and anthropic were taken into account.

Approach/Activities. This study counted on multiparameter analytical results (24 parameters) of 61 groundwater samples, collected from a monitoring network in an area of approximately 15 km2. For assessment of the geochemical equilibrium of each sample, hydrogeochemical modeling code PHREEQC was used, and the results of ionic balance between cations and anions and the results of the saturation indexes (SI) of each sample were taken into account. The results of ionic balance were used as the basis for validating the analytical results obtained, and the saturation indexes of each sample, to understand the precipitation or dissolution trends of each mineral of concern. For the three-dimensional modeling of multiparameter reactive transport, mathematical modeling code PHT3D was used, which, on its turn, was applied to obtain predictions of the evolution of the hydrogeochemical context for a period of 10 years from now.

Results/Lessons Learned. The multiparameter reactive transport model was built for two different scenarios: in (i) a current hydrogeochemical context was taken into account, encompassing natural and artificial source areas, but with no influence of the remediation process used for reduction in the concentration of barium and in (ii) a similar scenario was taken into account, but with continuous remediation efforts adopted. The assessment of the results obtained demonstrated a considerable influence of the remediation process used to reduce the concentrations of barium. It also demonstrated that in the older center of mass, the current barium concentrations, already below the reference standard, shall not go back to previous concentrations not even after interruption of the remediation system. On the other hand, the simulations indicated that in the most recent center of mass, the operation shall continue to avoid the spreading of a barium plume above the local background.