HYDROGEOCHEMICAL MODELING OF CONTAMINATED SOILS USING PHREEQC

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Abstract

Numerical modeling is an essential tool in chemical and environmental engineering. Computer simulations allow the mathematical solution of complex systems as well as the evaluation of the potential of new technologies. Computer simulations are useful to illustrate the main processes that take place in real cases and to evaluate the effects of the different parameters involved in a field-scale process, facilitating problem-based learning strategies.

In the present work, we present the experiences from including the software PHREEQC in the "Remediation of Contaminated Soil" course in the Chemical Engineering undergraduate degree. PHREEQC stands for "pH Reaction equilibrium", and it is a programming language that is designed to perform a wide variety of aqueous geochemical calculations.

During the course, the students have been introduced to the basic functionalities of the software in the computer lab. The students have used computer simulations to model multiphase and multi-species chemical systems, based on natural soils. In particular, the program has been used to quantify the chemical properties of the solid-liquid mixtures for different types of soils' nature and composition, with special emphasis on the matrix changes due to contamination. The students have also explored the simulation-based analysis of the soil properties changes due to the variation of external parameters, such as rain/drought cycles or the addition of chemicals. An introduction to reactive-transport processes was also possible using the software capabilities.

Parallelly, the students have been assigned small groups tasks, related to the study of a real case of soil contamination, with the aim of determine and design the most suitable remediation treatment. The evaluation of the knowledge acquisition about the software has been carried out based on how the students have used the software independently to model their own real-cases of soil contamination.

The simulation-based study of natural and contaminated soils has allowed the students to achieve a better understanding of the physical-chemical properties in those complex systems. Students have been able to do scenario analysis for selecting the appropriate remediation technique, as well as predict the remediation results. Furthermore, the student's satisfaction based on after-evaluation survey was very high. The students pointed out that the use of specialised software increased their interest on the course content, and that the new software skills are relevant in their curricula.

Keywords: Computer simulation, PHREEQC, problem-based learning, thermodynamics.