Simulation of Partitioning Tracers

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RESEARCH OBJECTIVES

Noble gases widely exist in nature, and except for radon, they are stable. Modern techniques can detect noble gases to relatively low concentrations and with great precision. In addition, different noble gases have different transport properties. These factors suggest that noble gases can be useful partitioning tracers for subsurface characterization. Previous research has shown that the solubility and dispersivity of a gas have strong temperature dependency, and that the dependency is gas-specific. We wanted to develop a numerical code that both simulates the transport of noble gases in the subsurface and also accounts for how temperature affects gas properties.

APPROACH

We base our code development on TOUGH2, a simulation code for multiphase, multicomponent, and heat flow. Among the many TOUGH2 modules, EOS7R specifically simulates two-phase, five-component flow and transport problems. The two phases are water and gas, and the five components are water, brine, air, and two radionuclides (Oldenburg and Pruess, 1995). For our studies, we added two subroutines to EOS7R and slightly modified the original code. One subroutine, called NOHEN, uses the laboratory-experiment-based Crovetto et al. (1982) model to calculate the Henry's law coefficient; the other, called GASDIF, uses the theoretical model given by Reid et al. (1987) to calculate noble gas diffusivity in the gas phase. At every time step and iteration, the program substitutes the most current temperature/pressure data to the two new subroutines to update the two coefficients for the next step of simulation.

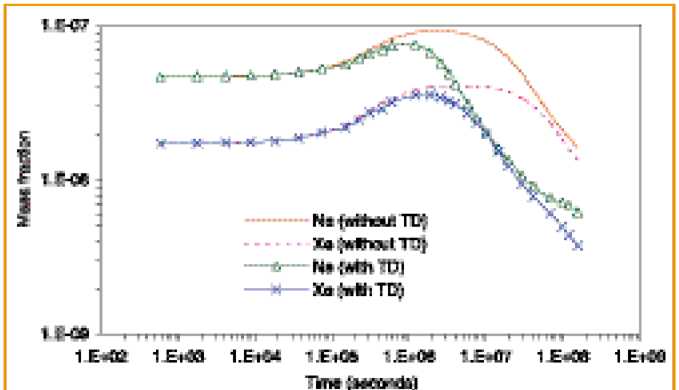

Figure 1. Noble gas mass fractions at the discharge face for example calculation.

ACCOMPLISHMENTS

A new fluid property module, EOSN, was developed for TOUGH2 to simulate transport of noble gases in the subsurface. Like most other sister modules, TOUGH2/EOSN can simulate nonisothermal multiphase flow and fully coupled transport in fractured porous media. In applying the new module, users need only to give the names of the two selected gases; all required thermodynamic properties are provided in an internal data bank. There are, however, options for users to overwrite internal molecular weights for modeling specific isotopes. Currently, six user-selectable gases are available: helium, neon, argon, krypton, xenon, and carbon dioxide. Radon may be added in the future; a capability to model radioactive decay by means of a half-life is already included in EOSN.

SIGNIFICANCE OF FINDINGS

Preliminary TOUGH2/EOSN simulations have shown that the temperature effect may play an important role in gas diffusion-dominant processes and in fluid exchange between matrix blocks and surrounding fractures. The difference in solubility and diffusivity between two different noble gases leads to a difference in resulting noble gas mass fractions (see Figure 1), which may provide additional information for subsurface studies. Vaporization and condensation of water may greatly affect mass fractions of gases, which is a factor to be considered in data analyses. The study of noble gases may be extended to any other noncondensable gases or even volatile organic chemicals (commonly referred to as VOCs).

RELATED PUBLICATIONS

Oldenburg, C. M., and K. Pruess, EOS7R: Radionuclide transport for TOUGH2. Berkeley Lab Report LBL-34868, 1995.

Shan, C., and K. Pruess, EOSN: A TOUGH2 module for noble gases. Berkeley Lab Report LBNL-52379, 2003.

ACKNOWLEDGMENTS

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