

# TOUGHREACT A COMPREHENSIVE NUMERICAL SIMULATOR FOR CHEMICALLY REACTIVE FLOWS

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## RESEARCH OBJECTIVES

Reactive chemical transport occurs in many geologic systems and environmental problems, including geothermal systems, diagenetic and weathering processes, subsurface waste disposal, acid mine drainage remediation, contaminant transport, and groundwater quality. The objective of this work was to develop a publicly available comprehensive simulation tool for these processes.

## APPROACH

The reactive transport simulator TOUGHREACT (Xu et al., 2004) has been developed by introducing reactive geochemistry into the existing framework of a nonisothermal, multi-component fluid and heat flow simulator TOUGH2. Our modeling of flow and transport in geologic media is based on space discretization by means of integral finite differences (IFD). The IFD method yields a flexible discretization for geologic media, one that allows use of irregular grids. This is well suited for simulation of flow, transport, and fluid-rock interaction in multi-region heterogeneous and fractured rock systems. An implicit time-weighting scheme is used for the individual components of the model, consisting of flow, transport, and kinetic geochemical reactions. TOUGHREACT uses a sequential iteration approach. Chemical transport is solved on a component basis, with the resulting concentrations obtained from the

transport substituted into the chemical reaction model. The system of chemical reaction equations is solved on a gridblock basis by a Newton-Raphson iteration. The chemical transport and reaction equations are iteratively solved until convergence.

## ACCOMPLISHMENTS

TOUGHREACT considers a wide variety of subsurface thermal-physical-chemical processes under various conditions of pressure, temperature, water saturation, ionic strength, and pH and Eh. It can be applied to one-, two-, or three-dimensional porous and fractured media with physical and chemical heterogeneity. The code can accommodate any number of chemical species present in liquid, gas, and solid phases. A variety of equilibrium chemical reactions are considered, such as aqueous complexation, gas dissolution/exsolution, cation exchange, and surface complexation. Mineral dissolution/precipitation can be simulated subject to either local equilibrium or kinetic controls, with coupling to changes in porosity and permeability. Chemical components can also undergo linear adsorption and radioactive decay. TOUGHREACT has been applied to a broad range of chemically reactive flow problems related to geothermal reservoir processes, groundwater protection, nuclear waste disposal, geologic storage of CO<sub>2</sub>, and mining engineering. This software was released to the public through the DOE Energy Science and Technology Software Center in November 2004.

## SIGNIFICANCE OF FINDINGS

TOUGHREACT is a very versatile simulator that can be applied to a broad range of environmental and resource problems of interest to DOE and industry.

## RELATED PUBLICATION

Xu, T., E.L. Sonnenthal, N. Spycher, and K. Pruess, TOUGHREACT User's Guide: A simulation program for non-isothermal multiphase reactive geochemical transport in variable saturated geologic media. Berkeley Lab Report LBNL-55460, 2004.

## ACKNOWLEDGMENTS

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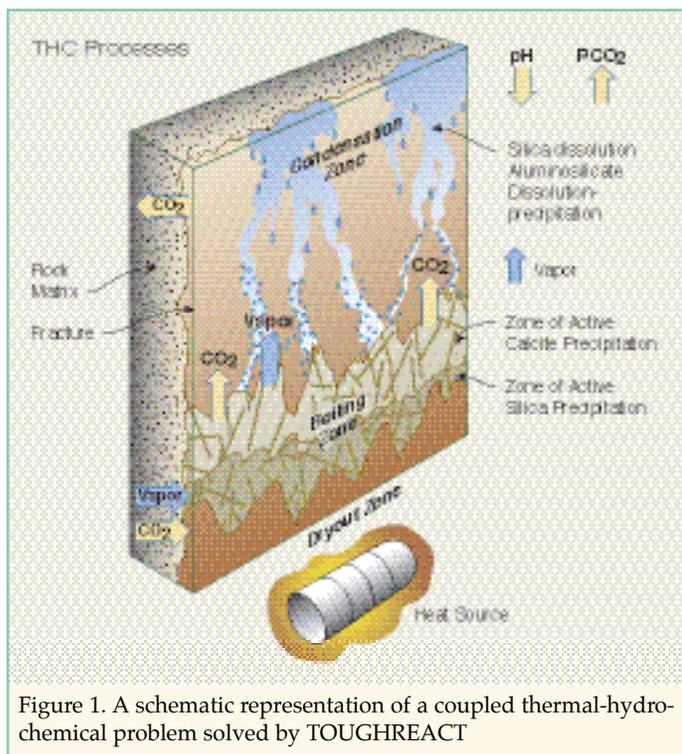


Figure 1. A schematic representation of a coupled thermal-hydro-chemical problem solved by TOUGHREACT