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TOUGHREACT—A simulation program for non-isothermal multiphase reactive geochemical transport in variably saturated geologic media: Applications to geothermal injectivity and CO_2 geological sequestration ☆

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Abstract

TOUGHREACT is a numerical simulation program for chemically reactive non-isothermal flows of multiphase fluids in porous and fractured media. The program was written in Fortran 77 and developed by introducing reactive geochemistry into the multiphase fluid and heat flow simulator TOUGH2. A variety of subsurface thermo-physical–chemical processes are considered under a wide range of conditions of pressure, temperature, water saturation, ionic strength, and pH and Eh. Interactions between mineral assemblages and fluids can occur under local equilibrium or kinetic rates. The gas phase can be chemically active. Precipitation and dissolution reactions can change formation porosity and permeability. The program can be applied to 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. Here we present two examples to illustrate applicability of the program. The first example deals with injectivity effects of mineral scaling in a fractured geothermal reservoir. A major concern in the development of hot dry rock and hot fractured rock reservoirs is achieving and maintaining adequate injectivity, while avoiding the development of preferential short-circuiting flow paths. Rock–fluid interactions and associated mineral dissolution and precipitation effects could have a major impact on the long-term performance of these reservoirs. We used recent European studies as a starting point to explore chemically induced effects of fluid circulation in the geothermal systems. We examine ways in which the chemical composition of reinjected waters can be modified to improve reservoir performance by maintaining or even enhancing injectivity. The second TOUGHREACT application example is related to CO_2 geologic sequestration in a saline aquifer. We performed numerical simulations for a commonly encountered Gulf Coast sediment under CO_2 injection conditions in order to analyze the impact of CO_2 immobilization through carbonate precipitation. Using the data presented in this paper, the CO_2 mineral-trapping capability after 10,000 years can reach 60 kg/m^3 of sandstone by secondary carbonate mineral precipitation such as

☆ Code is distributed to the public through the US Department of Energy's Energy Science and Technology Software Center (Email: estsc@adonis.osti.gov; WorldWideWeb: http://www.osti.gov/estsc/).

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siderite, ankerite, and dawsonite. Most of the simulated mineral alteration pattern is consistent with the field observations of natural CO_2 reservoirs.

Keywords: Reactive fluid flow; Geochemical transport; TOUGHREACT; Hydrothermal systems; Mineral scaling; Clay swelling; Injectivity enhancement; CO_2 geologic sequestration; Mineral trapping; Saline aquifer

1. Introduction

Coupled modeling of subsurface multiphase fluid and heat flow, solute transport, and chemical reactions can be applied to 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. TOUGHREACT is a numerical simulation program for reactive chemical transport that has been developed by introducing geochemistry into the existing framework of a non-isothermal multi-component fluid and heat flow simulator TOUGH2 (Pruess et al., 1999). A broad range of subsurface thermo-physical–chemical processes are considered under various thermo-hydrological and geochemical conditions of pressure, temperature, water saturation, ionic strength, and pH and Eh. TOUGHREACT 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, and cation exchange. Mineral dissolution/precipitation can take place subject to either local equilibrium or kinetic controls, with coupling to changes in porosity and permeability and capillary pressure in unsaturated systems. Chemical components can also be treated by linear adsorption and radioactive decay.

The TOUGHREACT program is distributed to the public through the US Department of Energy's Energy Science and Technology Software Center (Email: estsc@adonis.osti.gov; WorldWideWeb: http://www.osti.gov/estsc/). The distribution CD provides a README file, the source codes and input data files, and a comprehensive user's guide that includes sample problems addressing geothermal reservoirs and hydrothermal systems, nuclear waste isolation, groundwater quality, sequestration of carbon dioxide in saline aquifers, and supergene copper enrichment (Xu et al., 2004c). Additional information is available on the TOUGHREACT homepage, at http://www-esd.lbl.gov/TOUGHREACT/. The program makes use of "self-documenting" features. The input files for sample problems provide benchmarks for proper code installation, serve as a self-teaching tutorial in the use of TOUGHREACT, and provide templates to help jump-start new applications.

TOUGHREACT is written in FORTRAN 77. It has been tested on various computer platforms, including Microsoft Windows- and Linux-based PCs, SUN Ultrasparc systems, Compaq Alpha-based workstations, Apple Macintosh G4 and G5 computers, and IBM RISC System/6000 workstations. An effort was made to have the TOUGHREACT source code comply with the ANSIX3.9-1978 (FORTRAN 77) standard, and on most machines the code should compile and run without modifications. The computer memory required by TOUGHREACT depends on the problem size such as numbers of grid blocks, aqueous and gaseous species, and minerals. Parameter statements are used in INCLUDE files. More details are given in the TOUGHREACT manual (Xu et al., 2004c).

To illustrate the applicability of the TOUGHREACT, we present two examples: (1) mineral scaling during wastewater injection into a fractured geothermal reservoir and (2) CO_2 geological sequestration in a deep saline aquifer.

2. Main scope

TOUGHREACT is applicable to one-, two-, or three-dimensional geologic domains with physical and chemical heterogeneity and can be applied to a wide range of subsurface conditions. The temperature (T) and pressure (P) range is controlled by the applicable range of the chemical thermo-dynamic database, and the range of the equation of state module employed. For example, the range in the commonly used database of EQ3/6 (Wolery, 1992) is 0–300 °C, 1 bar below 100 °C, and water saturation pressure above 100 °C. Because the equilibrium constants are generally not as sensitive to pressure as to temperature, the program may be applied to pressures of several hundred bars (corresponding to depths of less than a few km). The temperature and pressure range is limited only by the thermo-dynamic database. Water saturation can vary from completely dry to fully water-saturated. Activity coefficients of charged aqueous species are computed using an extended Debye–Huckel equation and parameters derived by Helgeson et al. (1981). The model can deal with ionic strengths from dilute to moderately saline water