SOFTWARE VALIDATION PLAN AND SOFTWARE VALIDATION REPORT FOR TOUGHREACT VERSION 3.0

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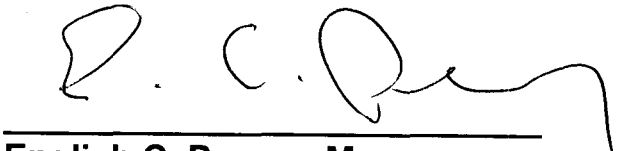

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1 SCOPE OF THE VALIDATION

This document establishes the software validation test plan for a full validation the installation and functionality of the non-isothermal reactive geochemical transport code TOUGHREACT Version 3.0 (Xu, et al., 2005). TOUGHREACT Version 3.0 is an acquired code, originally developed by the U.S. Department of Energy (DOE) Lawrence Berkeley National Laboratory. The software is used by staff at the Center for Nuclear Waste Regulatory Analyses (CNWRA) to provide technical assistance to the U.S. Nuclear Regulatory Commission (NRC) in its high-level waste program.

This software validation test plan applies to TOUGHREACT Version 3.0, and is intended to validate the software for use in modeling non-isothermal reactive geochemical transport processes as identified in the test cases described in Section 6. TOUGHREACT Version 3.0 will be placed under Technical Operation Procedure (TOP)–018 (CNWRA, 2005) configuration control when the validation activities outlined in Sections 6–9 have been completed.

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3 ENVIRONMENT

3.1 Software

TOUGHREACT Version 3.0 (Xu, et al., 2005) is a non-isothermal reactive geochemical transport code developed in FORTRAN 77 by Lawrence Berkeley National Laboratory to model transport processes in a wide variety of geologic systems including acid mine drainage remediation, contaminant transport, diagenetic and weathering processes, geothermal systems, groundwater quality, and subsurface waste disposal. The code can be applied to simulations of one-, two-, or three-dimensional porous and fractured media with physical and chemical heterogeneity. Both equilibrium and kinetically controlled reactions can be considered in the liquid, gas, and solid phases. The reactions include aqueous complexation, cation exchange, linear adsorption, radioactive decay, gas dissolution and exsolution, and mineral dissolution and precipitation. Chemical processes are coupled to changes in porosity, permeability, and capillary pressure in unsaturated systems. The developers have made an effort to have the

TOUGHREACT source code comply with ANSIX3.9–1978 and it should compile and run on most machines without modification. The code has been used on numerous computer platforms including Apple Macintosh computers, IBM-compatible personal computers, and Unix-based operating systems. This software validation test plan is designed to evaluate the installation and performance of TOUGHREACT Version 3.0 on an IBM-compatible personal computers with the Windows XP operating system (see Section 3.2).

3.2 Code Description

The code is run in batch mode in the DOS-operating environment. The following description of TOUGHREACT is based on the user's manual (Xu, et al., 2005) and a README text file provided with the TOUGHREACT Version 3.0 program. All file names are presented in italics throughout this report.

3.2.1 Input

TOUGHREACT requires three user-specified input files: *flow.inp*, *solute.inp*, and *chemical.inp*. The program also requires a thermodynamic database file that is specified in the *solute.inp* file. The database file contains reaction stoichiometries, equilibrium constants (log K), and regression coefficients of log K as a function of temperature. Additional elements, species, or phases can be added to the database if reaction stoichiometry, log K, and regression coefficients for the temperature dependence of log K are available. The three input files are described below.

flow.inp—Flow parameters. This file contains hydrogeologic information including porous and fractured media properties, flow grid information, time-stepping information, initial and boundary conditions, mass or heat sinks and sources, and data related to multi-phase fluid and heat flow. For larger and more complex problems, flow grid information, initial conditions, and mass or heat sinks and sources can be provided as separate files.

solute.inp—Transport parameters. This file contains parameters for reactive transport calculations including diffusion coefficients and configurations of model zones with different chemical compositions. The file also contains flags that control the printout of mineral and aqueous species and convergence criteria for solving the transport and chemical equations.

chemical.inp—Geochemical properties and parameters. This file contains the type and number of aqueous components, gases, minerals, and sorbed species. This file also includes the initial compositions of liquid, solid, and gas phases for each zone defined in *solute.inp*, along with kinetic data for mineral dissolution and precipitation (e.g., rate constants, surface areas).

3.2.2 Output

TOUGHREACT generates two types of output: fixed-name files, and user-specified name files. All output files can be viewed using a text editor program (e.g., Notepad or Wordpad) that is available as part of the Windows operating system.

3.2.2.1 Fixed-Name Output

flow.out—This file contains temperature, pressure, liquid saturation, mass flux, and phase velocity data for all grid blocks.

solute.out—This file is an echo of the input file *solute.inp* and includes transport parameters, chemical zone configurations, and other run-specific information.

chemical.out—This file is an echo of the input file *chemical.inp* and contains kinetic data, decay constants, and linear adsorption K_d values for designated species. This file also contains information read from the thermodynamic database including liquid, solid, and gas compositions; equilibrium constants; and reaction stoichiometries.

runlog.out—This file contains all run-related messages (e.g., error messages) and some run input parameters and is updated throughout a simulation.

chdump.out—This file contains the results of geochemical speciation, including mass balances, for each initial water composition in the *chemical.inp* file. Speciation data are also listed when convergence criteria are not reached for a grid block.

savechem—This file contains geochemical data that can be used to restart a simulation from the end of a previous run.

TOUGHREACT has two optional outputs: *mbalance.out*, which contains mass balance information; and *min_SI.dat*, which contains a mineral saturation index for each grid block at specified times.

3.2.2.2 User-Specified Output

These files must be specified by the user in the *solute.inp* file and are described in the required order below. The aqueous species, solid phase, and gas phase data files are in a TECPLOT-compatible format and contain time, grid coordinates, temperature, and the parameter for each file. Any file extension can be specified, however, the popular convention is to use a "*.dat*" extension. The data are outputs for all grid blocks at times specified in the *flow.inp* input file.

Iteration data—This file contains the number of iterations (chemical, flow, and transport) necessary to reach the specified convergence criteria at each timestep.

Aqueous species data—This file lists pH, gas and liquid saturations, and aqueous species concentrations. The number, type, and concentration units of species are specified in *solute.inp*.

Solid phase data—This file contains mineral abundances and exchanged species concentrations.

Gas phase data—This file contains gas partial pressures.

Plot data at specified grid blocks (time evolution)—This file contains an identified grid block, time temperature, pH, gas and liquid saturations, aqueous species concentrations, mineral abundances, exchanged species concentrations for grid blocks, and timesteps specified in the *solute.inp* file.

3.3 System Requirements and Installation

3.3.1 System Requirements

TOUGHREACT Version 3.0 is compatible with a variety of computer operating systems. The files on the program CD occupy about 40 megabytes of disk space. The amount of memory required to run TOUGHREACT Version 3.0 depends on the size and complexity of the problem. The developers have tested the program on the following computer platforms:

- Apple Macintosh G4 and G5 computers
- Compaq Alpha-based workstations
- IBM RISC system/6000 workstations
- Microsoft Windows- and Linux-based personal computers
- SUN Ultrasparc systems

3.3.2 TOUGHREACT Version 3.0 Installation

The following instructions are from the README.TXT file provided as part of the program CD. To install the software, simply copy all files from the program CD to the user's PC. The name of the target folder is specified by the user. The program CD contains the following folders and files (Table 3-1).

Additional instructions are provided in the README.TXT file for creating executable files for the other non-IBM PC operating systems. Creating executable files for other operating systems is beyond the scope of this validation plan. For informational purposes, the contents of the README.TXT file is presented in Appendix A.

4 PREREQUISITES

TOUGHREACT Version 3.0 runs on an IBM PC and requires that a thermodynamic database and three input files (*flow.inp*, *solute.inp*, and *chemical.inp*) be present in the same directory as the batch executable file. The user can choose from six executable files with different fluid flow modules. Additional details about the executable files are provided below (Table 4-1). Other than basic PC knowledge, the user does not need to alter any scripts or executable files.

Table 3-1. TOUGHREACT Version 3.0 Directory Structure	
Folder	**Folder Contents**
TOUGHREACT (user-specified folder name)	README.TXT
TOUGHREACT\documents	TOUGHREACT User's Manual
TOUGHREACT\EXE-files-PC	Executable files for IBM PC
TOUGHREACT\sample-problems	Input and output files for eight sample problems
TOUGHREACT\source-files	makefile and source files
TOUGHREACT\utility-programs	utility programs for the thermodynamic database

Table 4-1. TOUGHREACT Version 3.0 Precompiled Executable Files		
Executable File Name	**Phases Considered**	**Typical Applications/Problems**
treact_EOS1	water, water with tracer	environmental, hydrothermal
treact_EOS2	water, CO_2	environmental, hydrothermal
treact_EOS3	water, air	environmental, hydrothermal
treact_EOS4	water, air	same as EOS3 with VP lowering*
treact_EOS9	saturated-unsaturated flow of water	ambient temperature and pressure reactive geochemical transport
treact_ECO2	water, NaCl, CO_2	CO_2 disposal in deep brine aquifers
*Note: VP—vapor pressure lowering due to capillary pressure		

5 ASSUMPTIONS AND CONSTRAINTS

Reactive transport modeling requires the user to make many simplifications and assumptions. The factors controlling flow and transport must be captured along with the thermodynamic and kinetic controls for complex interactions among multiple chemical species in the solid, liquid, and gas phases. The mathematical relationships that describe flow, transport, and chemical processes are well understood. The results from reactive transport modeling are dependent on the type and quality of the data used in the simulation. For example, geochemical processes rely on a thermodynamic database and kinetic rate constants provided by the user. The TOUGHREACT program is generally applicable under the following conditions:

Temperature: 0 to 300 °C [32 to 572 °F]
Pressure: 1 to several hundred bars
Water saturation: completely dry to fully saturated

Ionic strength:	dilute to moderately saline (6 molal for NaCl system)
pH:	any value
Eh:	any value

Additional discussions on governing equations and simplifying TOUGHREACT approximations and solution methods can be found in the User's Guides for TOUGHREACT and TOUGH2 (Xu, et al., 2005; Pruess, et al., 1999). All users are encouraged to familiarize themselves with this information.

6 TEST CASES

Eight sample problems that were provided as part of the TOUGHREACT program disk were used as test cases for this validation. These problems are discussed in detail in the user's manual (Xu, et al., 2005) and include a comparison of model output with analytical solutions and field experimental data. The scope of the sample problems covers a wide range of geologic settings and environmental systems. All of the flow modules (ECO2, EOS1, EOS2, EOS3, EOS4, and EOS9) are demonstrated in the sample set. Each of the sample problems is discussed in detail below.

6.1 Test Input

The eight sample problems are supplied with input and output files (Xu, et al., 2005). The results of these validation test runs were compared to the supplied outputs. These results should be within four significant digits of the supplied outputs. The number of iterations required to reach convergence and the total run time may differ from the original output files. However, these differences should have no effect on the calculated results.

Each of the test problems requires a *flow.inp*, *solute.inp*, and *chemical.inp* file. For more complex simulations in addition to these three files, Problem 6.5 requires the following three files to be present. These files supersede information that is otherwise contained in the *flow.inp* file.

- GENER—list of mass or heat sinks or sources
- INCON—list of initial conditions for specific grid blocks
- MESH—list of grid blocks or volume elements

6.2 Test Procedure

Each of the example problems is located in its own folder within the TOUGHREACT\sample-problems directory. The input files must be transferred to a separate working folder because the program will over-write the existing output files. Folders and subdirectories can be created and files can be copied in a variety of ways using Windows XP or DOS commands from the command prompt window. A general set of instructions is provided below. The example scripts assume that TOUGHREACT files are located on the D:\drive.

- Create a folder for the validation test run (e.g., D:\TOUGHREACT\validation_test)
- Create a working folder for each example problem (e.g., D:\TOUGHREACT\validation_test\example_1)
- Copy *flow.inp*, *solute.inp*, and *chemical.inp* from the appropriate sample problem folder to the appropriate working directory
- Copy the appropriate executable and database file from the TOUGHREACT\EXE-files-PC folder to the working folder
- Open a command prompt window (In Windows XP the command prompt can be found by selecting *start/Programs/Accessories/Command Prompt*)
- Change the command prompt to the working directory using the "cd" command if necessary (e.g., D:\>cdTOUGHREACT\validation_test\example_1)
- Type in the executable file name and hit the enter key; the code will automatically read the input files (e.g., D:\TOUGHREACT\validation_test\example_1>treact_EOS9)

6.3 Test Results

As stated previously, the results of the test run should be within four significant digits of the supplied outputs from the TOUGHREACT manual (Xu, et al., 2005). The number of iterations required to reach convergence and the total run time could vary from the original output files. However, these difference should have no effect on the calculated results.

Three of the fixed-name output files (*flow.out*, *chemical.out*, and *solute.out*) and the four user specified-name output files were compared using the TextPad text editor program. For most comparisons, the validation test output files matched the outputs supplied as part of the program disk exactly. The results of the individual file comparisons are presented in Appendix B.

The validation testing was considered successful because there were no significant differences between the supplied outputs and the outputs generated as part of this validation plan. Below are the results of the validation output and output from the manual. Only one set of data results are presented due to the fact the numerical output is exactly the same.

6.3.1 Aqueous Transport With Adsorption (Linear K_d) and Decay—Module EOS9

This one-dimensional problem considers the movement of water and four chemical species through a fully water-saturated porous media. The species have varying distribution coefficients (K_d values) and half-lives. The objective of this problem is to demonstrate the use of linear distribution coefficients and decay constants. The results of this simulation are compared with an analytical solution to the problem (Javandel, et al., 1984).

With the exception of calculation time, the output files for this problem are identical to the files that accompany the program. A total of four species are simulated in a single run. Species 1 is not subject to adsorption (R = 1) and decay ($t_{1/2}$ = infinite), and is denoted by 'na^{+}' in chemical input file '*chemical.inp*'. Species 2 has R = 2 and $t_{1/2}$ = infinite, and is denoted by 'skdd1' in the chemical input file '*chemical.inp*'. Species 3 has a R = 1 and a $t_{1/2}$ = 20 days, and is denoted by 'skdd2' in the input file. Species 4 has R = 2 and $t_{1/2}$ = 20 days, and is denoted by 'skdd3' in the input file. Species skdd1, skdd2, and skdd3 are artificial tracer species. The species names must appear in the primary species block of the thermodynamic database. Initial concentrations for all four species are set equal to a very small value of 10^{-10} mol/l (practically zero, because TOUGHREACT uses log10 calculations for concentrations in order to avoid convergence problems). The inlet concentrations are set equal to 10^{-4} mol/l for all four species. An analytical solution for this problem is given in Javandel, et al. (1984). In the numerical simulation, we give a diffusion coefficient of zero. Dispersion is not considered in this code. The numerical results are listed in Figure 6-1. and are presented together with analytical solution from Javandel, et al. (1984) in Figure 6-2.

6.3.2 Water Quality in the Aquia Aquifer, Maryland—Module EOS9

This problem simulates a field-scale ambient aquifer system located adjacent to the Chesapeake Bay. The simulation considers Calcite dissolution and cation exchange among Na^{+} and Ca^{2+}, Mg^{2+}, and K^{+}. The objective of this problem is to demonstrate the use of cation exchange and mineral dissolution/precipitation. The simulation compares the field measurements (Chapelle and Knobel, 1983) that tracked the behavior of the above cations, pH, and alkalinity along a 112.7-km [70-mi] flow path from the recharge zone to the interface with Chesapeake Bay.

With the exception of calculation time, the output files for this problem are identical to the output of the example problems included with the program. Part of the output file for aqueous chemical concentrations is given in Figure 6-3.

The results after a simulation time of 144 thousand years are compared to observations of major cations and alkalinity (Figure 6-4). The agreement between numerical results and observations is reasonably satisfactory. An apparent dip in alkalinity is observed just before Na_{+} concentrations increase, which is matched by the simulation. The upstream increase of Ca^{2+} concentrations in the region where K^{+} and Mg^{2+} are at a peak indicates an increased concentration of Ca-X_2 (X represents cation exchange sites). The increase occurred during flushing of Na^{+} and is due to dissolution of calcite. The increase of Na^{+} and alkalinity at the downstream end agrees with earlier conclusions about the development of $NaHCO_3$ water quality in a freshening aquifer (Chapelle and Knobel, 1983).

X	SL	T	pH	na+	skdd1	skdd2	skdd3
0.000	1.0000	4.000	7.0035	0.1000E-03	0.1000E-03	0.9352E-04	0.8783E-04
0.000	1.0000	4.000	7.0035	0.1000E-03	0.1000E-03	0.8746E-04	0.7714E-04
0.000	1.0000	4.000	7.0035	0.1000E-03	0.9996E-04	0.8180E-04	0.6775E-04
0.000	1.0000	4.000	7.0035	0.1000E-03	0.9983E-04	0.7650E-04	0.5948E-04
0.000	1.0000	4.000	7.0035	0.1000E-03	0.9943E-04	0.7154E-04	0.5218E-04
0.000	1.0000	4.000	7.0035	0.1000E-03	0.9844E-04	0.6690E-04	0.4567E-04
0.000	1.0000	4.000	7.0035	0.1000E-03	0.9640E-04	0.6257E-04	0.3979E-04
0.000	1.0000	4.000	7.0035	0.1000E-03	0.9280E-04	0.5852E-04	0.3437E-04
0.000	1.0000	4.000	7.0035	0.9999E-04	0.8724E-04	0.5472E-04	0.2931E-04
0.000	1.0000	4.000	7.0035	0.9997E-04	0.7957E-04	0.5117E-04	0.2454E-04
0.000	1.0000	4.000	7.0035	0.9993E-04	0.7006E-04	0.4785E-04	0.2006E-04
0.000	1.0000	4.000	7.0035	0.9983E-04	0.5929E-04	0.4473E-04	0.1593E-04
0.000	1.0000	4.000	7.0035	0.9963E-04	0.4810E-04	0.4180E-04	0.1225E-04
0.000	1.0000	4.000	7.0034	0.9926E-04	0.3735E-04	0.3903E-04	0.9085E-05
0.000	1.0000	4.000	7.0034	0.9860E-04	0.2774E-04	0.3639E-04	0.6490E-05
0.000	1.0000	4.000	7.0034	0.9753E-04	0.1970E-04	0.3385E-04	0.4458E-05
0.000	1.0000	4.000	7.0034	0.9590E-04	0.1338E-04	0.3137E-04	0.2944E-05

Figure 6-1. Part of Aqueous Concentrations Output File (*kdd_conc.dat*) for Problem of Aqueous Transport with Kd Adsorption and Decay After 50 Days (0.136893 yr). Figure from Xu ,et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

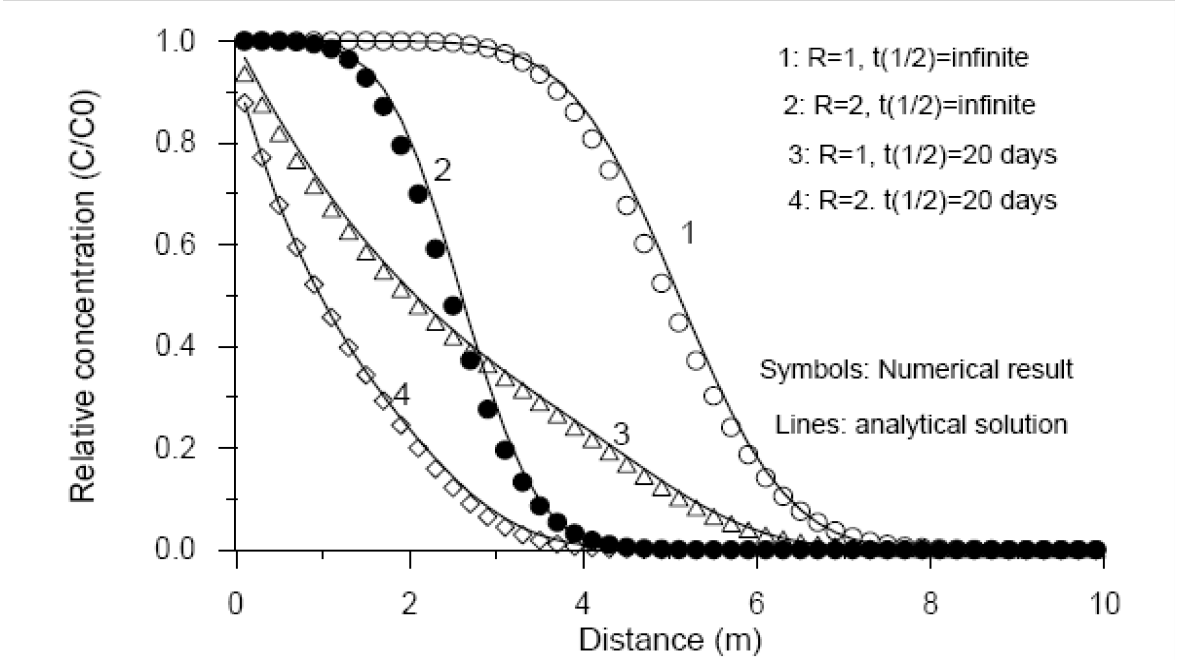

Figure 6-2. Relative Concentrations at 50 Days for 1-D Aqueous Solute Transport with Adsorption (Linear Kd) and Decay (Concentrations are Normalized to the Inlet Concentration of 10^{-4} mol/l). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

X	pH	ca+2	mg+2	na+	k+	hco3-
6.000	7.5732	0.1896E-02	0.2059E-03	0.1024E-03	0.6390E-04	0.3482E-02
10.000	7.6255	0.1679E-02	0.4146E-03	0.1060E-03	0.8174E-04	0.3457E-02
14.000	7.6944	0.1431E-02	0.6458E-03	0.1136E-03	0.1123E-03	0.3428E-02
18.000	7.7647	0.1218E-02	0.8268E-03	0.1295E-03	0.1596E-03	0.3396E-02
22.000	7.8237	0.1067E-02	0.9204E-03	0.1622E-03	0.2262E-03	0.3357E-02
26.000	7.8718	0.9625E-03	0.9315E-03	0.2284E-03	0.3116E-03	0.3304E-02
30.000	7.9205	0.8715E-03	0.8768E-03	0.3615E-03	0.4101E-03	0.3228E-02
34.000	7.9873	0.7616E-03	0.7636E-03	0.6250E-03	0.5048E-03	0.3120E-02
38.000	8.1005	0.6014E-03	0.5861E-03	0.1135E-02	0.5591E-03	0.2982E-02
42.000	8.3289	0.3638E-03	0.3355E-03	0.2071E-02	0.5028E-03	0.2846E-02
46.000	8.6983	0.1559E-03	0.1325E-03	0.3160E-02	0.3052E-03	0.2865E-02
50.000	8.8841	0.9860E-04	0.8024E-04	0.3727E-02	0.1911E-03	0.3062E-02
54.000	8.8642	0.9453E-04	0.7704E-04	0.4115E-02	0.1641E-03	0.3402E-02
58.000	8.7679	0.1042E-03	0.8612E-04	0.4562E-02	0.1676E-03	0.3898E-02
62.000	8.6654	0.1169E-03	0.9800E-04	0.5062E-02	0.1799E-03	0.4470E-02
66.000	8.5999	0.1256E-03	0.1065E-03	0.5433E-02	0.1900E-03	0.4894E-02

Figure 6-3. Part of Aqueous Concentrations Output File (*aqui_con.dat*) for Problem of Water Quality in Aquia Aquifer after 144 × 10^6 years. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

6.3.3 Infiltration and Calcite Deposition at Yucca Mountain, Nevada—Module EOS3

This problem simulates flow and transport through the chemically and structurally complex unsaturated zone at Yucca Mountain, Nevada (Xu, et al., 2003). The objective of this simulation is to demonstrate the proper treatment of the following hydrological and geochemical processes:

- Infiltration
- Geothermal gradient
- Gaseous CO_2 diffusion and partitioning between gas and liquid
- Fracture-matrix interactions (fluid flow and chemical constituents)
- Water-rock interaction

The results of this simulation are compared to bulk rock calcite abundances measured by the U.S. Geological Survey (Bechtel SAIC Company, LLC, 2001).

The calculation time of the *flow.out* file is the only difference between output files; other than that the output files for this problem are identical to the output of the example problems included with the program. Parts of the output files for aqueous chemical concentrations and changes of mineral abundances are given in Figures 6-5 and 6-6.

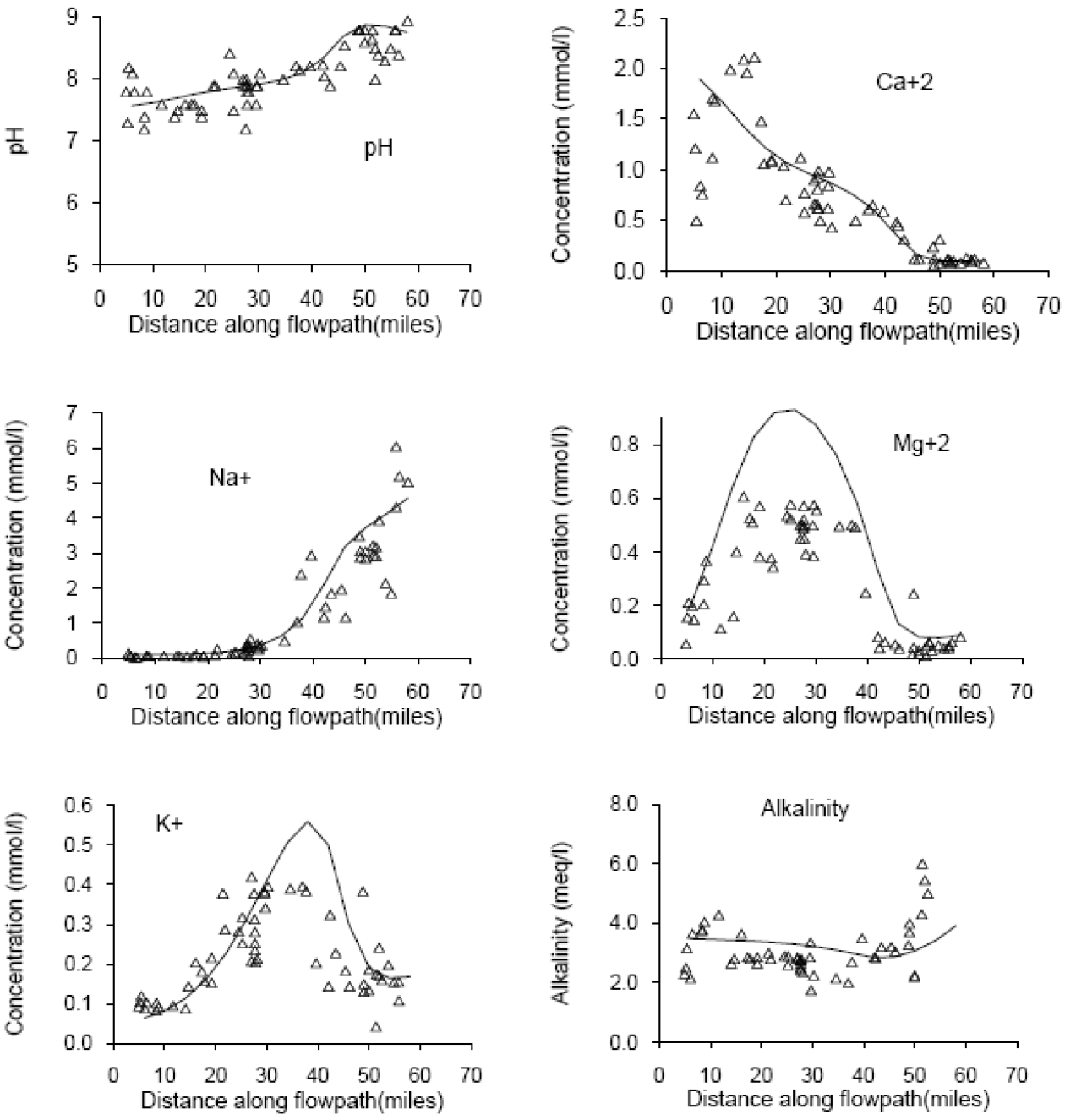

Figure 6-4. Concentrations of Na^{+}, K^{+}, Mg^{2+}, Ca^{2+}, Alkalinity, and pH Along a Flow Path in the Aquia Aquifer (Maryland). Symbols Indicate Observations Provided by Appelo (1994) and Originally from Chapelle and Knobel (1983); Solid Lines Represent Simulated Concentrations Using TOUGHREACT. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

Z	SL	T	pH	ca+2	na+	sio2(aq)	hco3-
1482.000	0.0338	15.750	8.1986	0.2258E-02	0.2666E-02	0.1232E-02	0.2853E-02
1482.000	0.2965	15.750	8.1992	0.2258E-02	0.2666E-02	0.1236E-02	0.2850E-02
1449.000	0.0172	16.022	8.1422	0.2373E-02	0.2665E-02	0.1401E-02	0.3084E-02
1449.000	0.9938	16.022	8.1385	0.2382E-02	0.2665E-02	0.1402E-02	0.3101E-02
1422.000	0.0302	16.290	8.1122	0.2402E-02	0.2665E-02	0.1292E-02	0.3148E-02
1422.000	0.8104	16.290	8.1123	0.2402E-02	0.2665E-02	0.1292E-02	0.3148E-02
1413.000	0.0422	16.448	8.1080	0.2404E-02	0.2665E-02	0.1201E-02	0.3155E-02
1413.000	0.8338	16.448	8.1080	0.2404E-02	0.2665E-02	0.1194E-02	0.3155E-02
1404.000	0.0254	16.680	8.1038	0.2394E-02	0.2665E-02	0.1182E-02	0.3135E-02
1404.000	0.3328	16.680	8.1037	0.2393E-02	0.2665E-02	0.1181E-02	0.3134E-02
1396.000	0.0307	16.940	8.1034	0.2396E-02	0.2665E-02	0.1185E-02	0.3140E-02
1396.000	0.6580	16.940	8.1034	0.2397E-02	0.2665E-02	0.1185E-02	0.3140E-02
1370.000	0.0246	17.425	8.0991	0.2398E-02	0.2665E-02	0.1181E-02	0.3143E-02
1370.000	0.6159	17.425	8.0991	0.2398E-02	0.2665E-02	0.1181E-02	0.3143E-02
1344.000	0.0205	17.995	8.0956	0.2391E-02	0.2664E-02	0.1180E-02	0.3128E-02
1344.0	0.4469	17.995	8.0956	0.2391E-02	0.2664E-02	0.1180E-02	0.3128E-02

Figure 6-5. Part of File *YMC_conc.dat* for Problem No. 3 after t = 100 yr (SL is Water Saturation, T is Temperature in °C, Unit of Concentrations is mol/l). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

Z	calcite	tridymite	cristoba-a	quartz	sio2(amor.)	glass
1482.000	0.2211E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.2534E-11
1482.000	0.8814E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.1578E-06
1449.000	0.1457E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.9484E-12
1449.000	0.3226E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.5826E-06
1422.000	0.2566E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.2292E-11
1422.000	0.6886E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.4819E-06
1413.000	0.3417E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.4365E-11
1413.000	0.1345E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.5208E-07
1404.000	0.2255E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.3221E-11
1404.000	0.7170E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.2129E-07
1396.000	0.2839E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.3078E-10
1396.000	0.7281E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.6026E-07
1370.000	0.2325E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.8919E-12
1370.000	0.1116E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.5302E-07
1344.000	0.2074E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.5255E-11
1344.000	0.1059E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	-0.4486E-07

Figure 6-6. Part of File *YMC_min.dat* for Problem No. 3 after t = 100 yr, Giving Changes in Mineral Abundances (in Volume Fraction, Positive Values Indicate Precipitation and Negative Dissolution). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

The simulated total (fracture plus matrix) calcite abundances in the WT–24 column for three infiltration rates, together with U.S. Geological Survey measured data, are presented in Figure 6-7. In general, the results obtained using the base-case infiltration rate {5.92 mm/yr [0.02 –ft/yr]} agree more closely with the measured WT–24 calcite abundances than those obtained using the other infiltration rates.

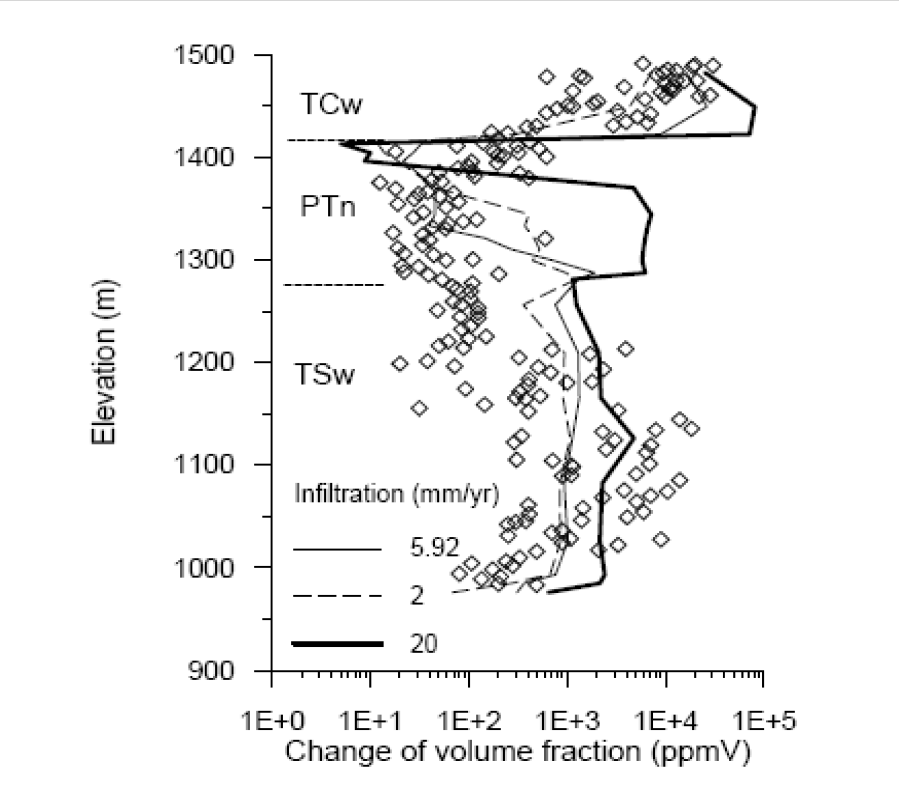

Figure 6-7. Simulated Total (Fracture Plus Matrix) Calcite Abundances (Volume Fraction) in the WT–24 Column for Different Infiltration Rates after 10 Million Years (Extended Geochemical System). Diamonds Represent Bulk Rock Calcite Abundances Measured by the U.S. Geological Survey (Paces, et al., 2001). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

6.3.4 Heater Test Problem—Module EOS4

This problem simulates a drift-scale thermal test at Yucca Mountain, Nevada. The objective of this two-dimension simulation is to demonstrate the following coupled thermal, hydrological, and chemical processes:

- Time-dependant heat generation
- Dual permeability
- Vapor pressure lowering
- Several aqueous, gaseous, and mineral species
- CO_2 diffusion (temperature- and pressure-dependent)
- Coupling of permeability and capillary pressure-to-porosity changes

The results of this simulation are compared to data collected during the drift-scale heater test at the Yucca Mountain site (Bechtel SAIC, LLC, 2005).

The calculation time and the number of iterations of the *flow.out* and *Iter.dat* files are the only differences; other than that the output files for this problem are identical to the output of the example problems included with the program. Parts of the output files for aqueous chemical concentrations and changes of mineral abundances are given in Figures 6-8 and 6-9.

A few comparisons that compare model vs measured results for CO_2 and pH over the duration of the study are presented below. Aqueous species in waters collected in the drift-scale heater test exhibit small reductions in pH, from about pH 8 in the pore water to about 6–8 in condensate waters. The drop in pH is related to the local increases in C_2 concentrations. Figure 6-10 is an example of the initial drop in pH during vapor condensation, followed by increasing pH as the zone is further heated and CO_2 is diluted by water vapor. Figure 6-11 shows the Modeled gas phase CO_2 concentrations in fractures after 3 years and the relative borehole locations. Comparisons of modeled CO_2 concentrations to measurements performed on gas samples from various boreholes are presented in Figure 6-12. Simulated and measured concentrations are close in magnitude and in their trends. There is little difference between fracture and matrix concentrations, because of rapid equilibration by advection and diffusion of gas species and their local equilibration with pore water.

6.3.5 CO_2 Disposal in Deep Saline Aquifers—Module ECO2

This one-dimensional radial flow problem (Pruess, et al., 2003) simulates the injection of CO_2 into a homogeneous porous media containing 1 M NaCl brine. The objective of this simulation is to demonstrate the ability of the ECO2 module to model the chemical reactions that would take place when CO_2 at high pressures comes in contact with various mineral assemblages in the presence of brine. This simulation provides predictions of water saturation, mineral abundances, and cumulative CO_2 sequestration as a function of distance from the injection well for various times.

The output files for this problem are identical to the output of the example problems included with the program. However, the *flow.out* was not included with the initial files so a comparison is not possible. Parts of the output files for fluid flow, aqueous chemical concentrations, and changes of mineral abundances are given in Figures 6-13, 6-14, and 6-15. These data correlate to the graphical representations of water saturation, change in mineral abundance, and CO_2 sequestered versus distance for various time period with in the run (Figures 6-16, 6-17, and 6-18).

6.3.6 Supergene Copper Enrichment—Module EOS9

This problem simulates supergene copper enrichment where metals are weathered and transported from a near-surface oxidizing zone and deposited as secondary ore compounds under reducing conditions at depth. This simulation is based on field and laboratory studies by Brimhall, et al. (1985) and Alpers and Brimhall (1989) and considers saturated and unsaturated liquid flow, diffusive oxygen transport, and kinetically controlled dissolution and precipitation of minerals. The objective of this simulation is to demonstrate the multiple interacting continua method to resolve the flow and diffusion of chemicals between fractures and solid matrix and the use of kinetic rate constants and reactive surface areas to model geochemical processes and transport. This simulation provides predictions of changes in mineral abundances (dissolution and precipitation) in the rock matrix as a function of distance from the fracture.

X	Z	pH	ca+2	mg+2	na+	sio2(aq)	hco3-
1.999	-1.534	8.3457	0.2441E-02	0.6970E-03	0.2835E-02	0.1205E-02	0.3102E-02
1.999	-1.534	8.3242	0.2484E-02	0.6940E-03	0.2823E-02	0.1200E-02	0.3204E-02
2.039	-1.565	8.3439	0.2441E-02	0.6942E-03	0.2830E-02	0.1203E-02	0.3111E-02
2.039	-1.565	8.3239	0.2484E-02	0.6933E-03	0.2828E-02	0.1202E-02	0.3205E-02
2.102	-1.613	8.3409	0.2446E-02	0.6932E-03	0.2828E-02	0.1202E-02	0.3124E-02
2.102	-1.613	8.3230	0.2484E-02	0.6929E-03	0.2828E-02	0.1202E-02	0.3207E-02
2.182	-1.674	8.3374	0.2452E-02	0.6929E-03	0.2827E-02	0.1202E-02	0.3138E-02
2.182	-1.674	8.3220	0.2486E-02	0.6928E-03	0.2827E-02	0.1202E-02	0.3211E-02
2.261	-1.735	8.3344	0.2458E-02	0.6928E-03	0.2827E-02	0.1202E-02	0.3150E-02
2.261	-1.735	8.3210	0.2487E-02	0.6927E-03	0.2827E-02	0.1203E-02	0.3214E-02
2.340	-1.796	8.3317	0.2462E-02	0.6928E-03	0.2827E-02	0.1202E-02	0.3161E-02
2.340	-1.796	8.3200	0.2488E-02	0.6927E-03	0.2827E-02	0.1203E-02	0.3216E-02
2.459	-1.887	8.3284	0.2468E-02	0.6928E-03	0.2827E-02	0.1202E-02	0.3174E-02
2.459	-1.887	8.3188	0.2489E-02	0.6927E-03	0.2827E-02	0.1203E-02	0.3219E-02
2.618	-2.009	8.3249	0.2474E-02	0.6928E-03	0.2827E-02	0.1202E-02	0.3187E-02
2.618	-2.009	8.3175	0.2490E-02	0.6927E-03	0.2827E-02	0.1203E-02	0.3222E-02
2.777	-2.131	8.3221	0.2479E-02	0.6927E-03	0.2827E-02	0.1202E-02	0.3197E-02
2.777	-2.131	8.3164	0.2491E-02	0.6927E-03	0.2827E-02	0.1203E-02	0.3224E-02
2.975	-2.283	8.3195	0.2483E-02	0.6927E-03	0.2827E-02	0.1202E-02	0.3206E-02
2.975	-2.283	8.3153	0.2492E-02	0.6926E-03	0.2827E-02	0.1203E-02	0.3226E-02
3.213	-2.465	8.3170	0.2486E-02	0.6927E-03	0.2827E-02	0.1202E-02	0.3214E-02
3.213	-2.465	8.3141	0.2493E-02	0.6926E-03	0.2827E-02	0.1203E-02	0.3228E-02
3.768	-2.892	8.3135	0.2490E-02	0.6927E-03	0.2827E-02	0.1203E-02	0.3223E-02
3.768	-2.892	8.3122	0.2493E-02	0.6926E-03	0.2827E-02	0.1203E-02	0.3229E-02

Figure 6-8. Part of File *tec_conc.dat* for Problem No. 4, Giving Concentrations (mol/l) of Aqueous Components after t = 0.237909 yr. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

X	Z,	hematite	calcite	microcline	albite-low	anorthite
1.999	-1.534	-0.3454E-16	0.2282E-05	-0.3215E-08	-0.1233E-07	-0.3164E-11
1.999	-1.534	-0.6890E-16	0.1237E-06	0.2175E-05	-0.2397E-05	-0.4152E-08
2.039	-1.565	-0.4774E-16	0.2019E-05	-0.3345E-08	-0.1232E-07	-0.3165E-11
2.039	-1.565	-0.5320E-16	0.1205E-06	0.1858E-05	-0.2110E-05	-0.4154E-08
2.102	-1.613	-0.4842E-16	0.1768E-05	-0.3367E-08	-0.1225E-07	-0.3148E-11
2.102	-1.613	-0.5467E-16	0.1162E-06	0.1824E-05	-0.2080E-05	-0.4157E-08
2.182	-1.674	-0.4402E-16	0.1519E-05	-0.3340E-08	-0.1210E-07	-0.3109E-11
2.182	-1.674	-0.5667E-16	0.1118E-06	0.1821E-05	-0.2079E-05	-0.4160E-08
2.261	-1.735	-0.3899E-16	0.1309E-05	-0.3300E-08	-0.1192E-07	-0.3062E-11
2.261	-1.735	-0.5850E-16	0.1082E-06	0.1821E-05	-0.2079E-05	-0.4163E-08
2.340	-1.796	-0.3416E-16	0.1132E-05	-0.3254E-08	-0.1173E-07	-0.3011E-11
2.340	-1.796	-0.6029E-16	0.1052E-06	0.1820E-05	-0.2080E-05	-0.4167E-08
2.459	-1.887	-0.2910E-16	0.9145E-06	-0.3181E-08	-0.1143E-07	-0.2933E-11
2.459	-1.887	-0.6318E-16	0.1016E-06	0.1820E-05	-0.2080E-05	-0.4171E-08
2.618	-2.009	-0.2434E-16	0.6964E-06	-0.3091E-08	-0.1106E-07	-0.2838E-11
2.618	-2.009	-0.6659E-16	0.9829E-07	0.1819E-05	-0.2081E-05	-0.4176E-08
2.777	-2.131	-0.2051E-16	0.5358E-06	-0.3008E-08	-0.1072E-07	-0.2752E-11
2.777	-2.131	-0.6980E-16	0.9599E-07	0.1818E-05	-0.2081E-05	-0.4181E-08
2.975	-2.283	-0.1731E-16	0.3919E-06	-0.2918E-08	-0.1037E-07	-0.2660E-11
2.975	-2.283	-0.7352E-16	0.9417E-07	0.1817E-05	-0.2082E-05	-0.4187E-08
3.213	-2.465	-0.1481E-16	0.2715E-06	-0.2819E-08	-0.9988E-08	-0.2563E-11
3.213	-2.465	-0.7794E-16	0.9294E-07	0.1816E-05	-0.2082E-05	-0.4192E-08
3.768	-2.892	-0.1278E-16	0.1259E-06	-0.2631E-08	-0.9312E-08	-0.2389E-11
3.768	-2.892	-0.8508E-16	0.9239E-07	0.1815E-05	-0.2083E-05	-0.4202E-08

Figure 6-9. Part of File *tec_min.dat* for Problem No. 4, Giving Changes in Mineral Abundances (in Volume Fraction, Positive Values Indicate Precipitation and Negative Dissolution) after t = 0.237909 yr. Figure from Xu et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

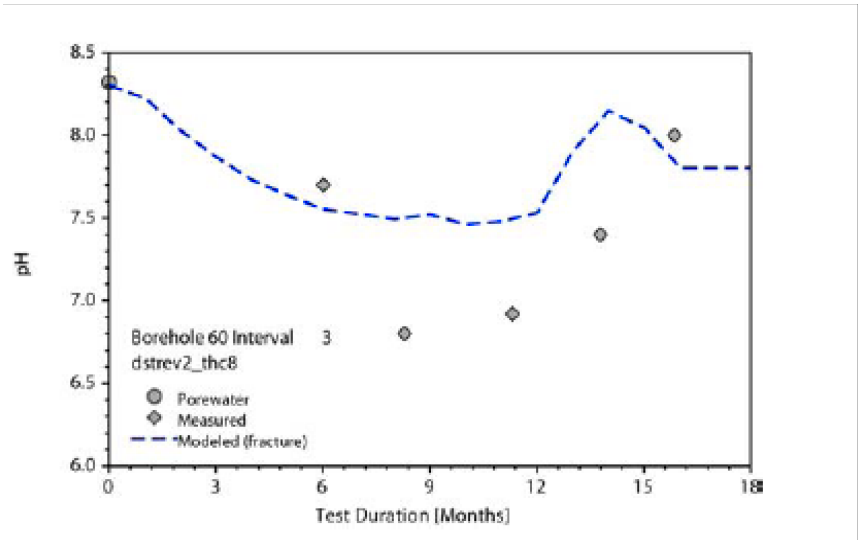

Figure 6-10. Measured and Modeled pH (in Fractures) for Samples Collected from Borehole Interval 60-3, Located Below the Heaters. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

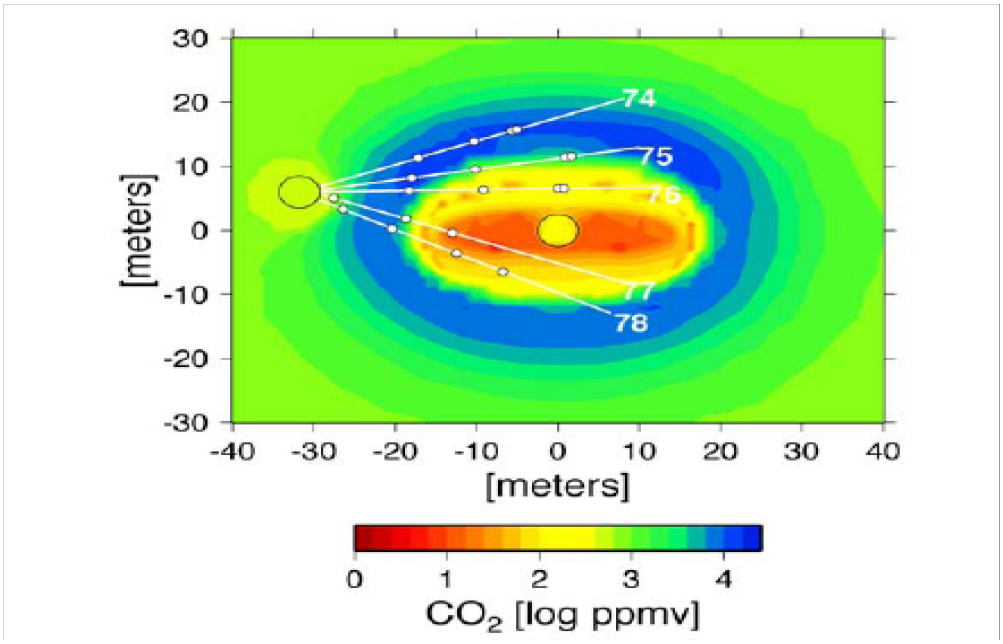

Figure 6-11. Borehole Positions. Modeled Gas Phase CO_2 Concentrations in Fractures after 3 Years of Heating. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

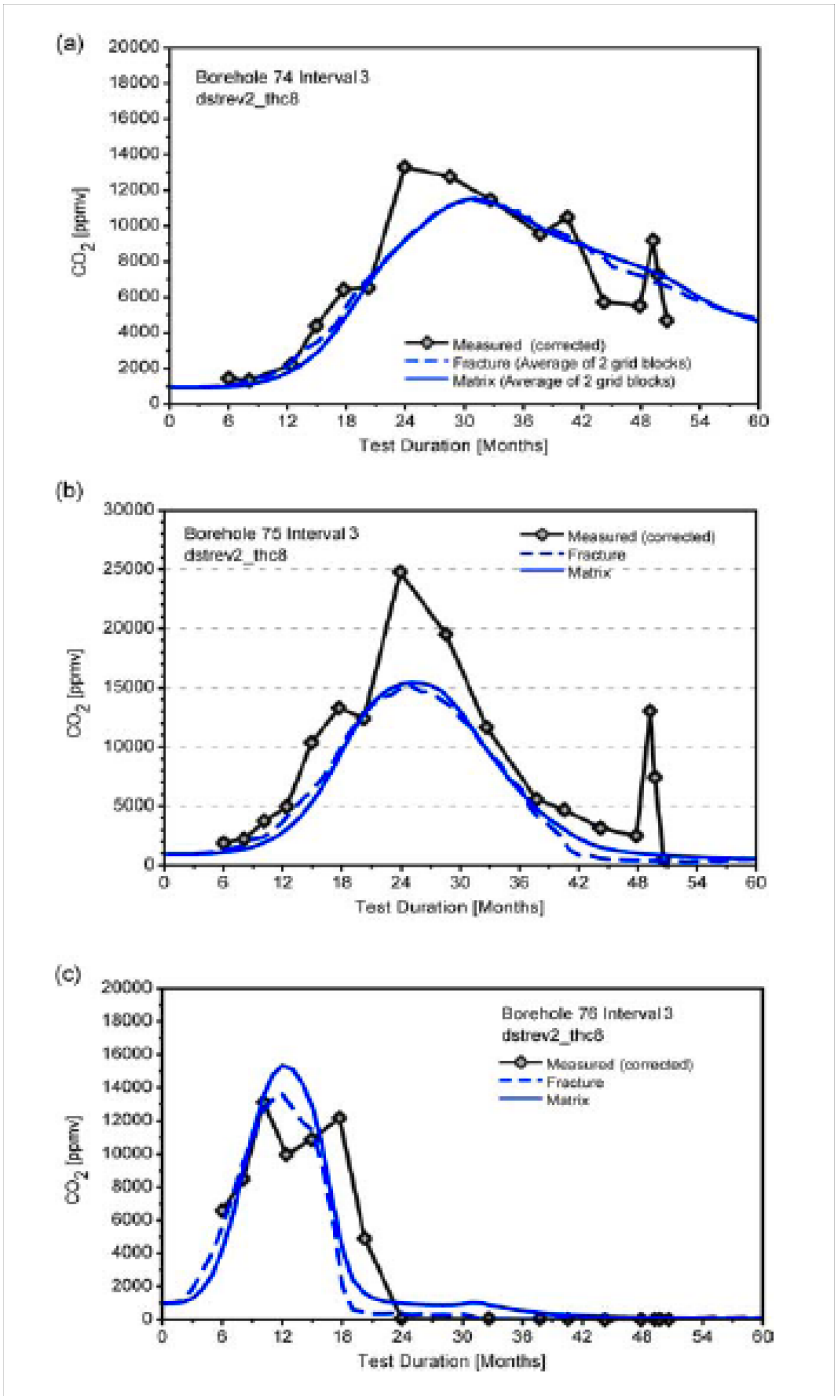

Figure 6-12. Modeled CO_2 Concentrations in Fractures and Matrix Compared to Measured Values From Boreholes (Corrected for Vapor Condensation) (a) Borehole interval 74-3 (Average of Bounding Grid Blocks); (b) Borehole Interval 75-3; (c) Borehole Interval 76-3. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

```
A1 1( 1, 3) ST = 0.100000E+01 DT = 0.100000E+01 DX1= 0.130721E+07 DX2= -.683215E-03
A1 2( 2, 3) ST = 0.300000E+01 DT = 0.200000E+01 DX1= 0.423626E+06 DX2= -.149300E-04
A1 2( 3, 3) ST = 0.400000E+01 DT = 0.100000E+01 DX1= 0.130134E+06 DX2= -.995983E-05
A1 2( 4, 7) ST = 0.600000E+01 DT = 0.200000E+01 DX1= 0.394548E+06 DX2= -.283532E-04
A1 2 5, 4) ST = 0.800000E+01 DT = 0.200000E+01 DX1= 0.217021E+06 DX2= -.297228E-04
---------------------------
OUTPUT DATA AFTER ( 328, 5)-2-TIME STEPS
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
TOTAL TIME KCYC ITER ITERC KON DX1M DX2M
0.315576E+09 328 5 2213 2 0.85171E+05 0.80346E-01
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
ELEM. IND. P T SG SS XNACL XCO2G
(Pa) (deg.C)
A1 1 1 0.27244E+08 75.00 0.98154E+00 0.18458E-01 0.00000E+00 0.10000E+01
A1 2 2 0.27095E+08 75.00 0.98687E+00 0.13125E-01 0.00000E+00 0.10000E+01
A1 3 3 0.27023E+08 75.00 0.98757E+00 0.12428E-01 0.00000E+00 0.10000E+01
A1 4 4 0.26975E+08 75.00 0.98760E+00 0.12405E-01 0.00000E+00 0.10000E+01
A1 5 5 0.26938E+08 75.00 0.98795E+00 0.12046E-01 0.00000E+00 0.10000E+01
```

Figure 6-13. Part of File *flow.out* for Problem No. 5 (CO_2 Disposal). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

X	pH	ca+2	mg+2	na+	k+	fe+2
15.860	0.5501E+01	0.6890E-02	0.1345E-11	0.4347E+01	0.7346E-04	0.3012E-03
16.760	0.5177E+01	0.1708E-01	0.1572E-14	0.1064E+01	0.2719E-04	0.3156E-03
17.700	0.5170E+01	0.1735E-01	0.1294E-14	0.1012E+01	0.2642E-04	0.3124E-03
18.670	0.5170E+01	0.1735E-01	0.1289E-14	0.1011E+01	0.2641E-04	0.3104E-03
19.690	0.5170E+01	0.1735E-01	0.1287E-14	0.1011E+01	0.2641E-04	0.3087E-03
20.740	0.5170E+01	0.1735E-01	0.1286E-14	0.1011E+01	0.2641E-04	0.3071E-03
21.830	0.5170E+01	0.1735E-01	0.1284E-14	0.1011E+01	0.2641E-04	0.3057E-03
22.960	0.5170E+01	0.1735E-01	0.1283E-14	0.1010E+01	0.2641E-04	0.3042E-03
24.130	0.5170E+01	0.1735E-01	0.1281E-14	0.1010E+01	0.2641E-04	0.3028E-03
25.350	0.5170E+01	0.1735E-01	0.1280E-14	0.1010E+01	0.2641E-04	0.3015E-03
26.620	0.5170E+01	0.1734E-01	0.1279E-14	0.1010E+01	0.2641E-04	0.3002E-03
27.930	0.5170E+01	0.1734E-01	0.1278E-14	0.1010E+01	0.2641E-04	0.2989E-03
29.300	0.5170E+01	0.1734E-01	0.1277E-14	0.1010E+01	0.2641E-04	0.2977E-03
30.710	0.5170E+01	0.1734E-01	0.1276E-14	0.1010E+01	0.2641E-04	0.2965E-03
32.180	0.5170E+01	0.1734E-01	0.1274E-14	0.1010E+01	0.2641E-04	0.2952E-03
33.710	0.5170E+01	0.1734E-01	0.1273E-14	0.1010E+01	0.2641E-04	0.2941E-03

Figure 6-14. Part of File *co2d_conc.dat* for Problem No. 5 after t = 10 yr. (For Coordinates from x = 0.15 to x = 14.99, Concentrations of Aqueous Species are Marked as "0.0000E+00" that Indicates a Zero Water Saturation, Which Are Not Shown Here). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

X	calcite	quartz	kaolinite	illite	oligoclase	smectite-na
15.860	-0.1705E-04	0.1268E-03	0.2918E-03	0.5074E-04	-0.1450E-02	0.8274E-03
16.760	-0.7417E-04	0.1302E-03	0.3116E-03	0.5146E-04	-0.1536E-02	0.8785E-03
17.700	-0.8320E-04	0.1322E-03	0.3169E-03	0.5190E-04	-0.1560E-02	0.8928E-03
18.670	-0.7321E-04	0.1336E-03	0.3199E-03	0.5232E-04	-0.1575E-02	0.9021E-03
19.690	-0.7158E-04	0.1348E-03	0.3226E-03	0.5273E-04	-0.1589E-02	0.9102E-03
20.740	-0.6991E-04	0.1359E-03	0.3253E-03	0.5314E-04	-0.1602E-02	0.9179E-03
21.830	-0.5221E-04	0.1370E-03	0.3278E-03	0.5355E-04	-0.1615E-02	0.9252E-03
22.960	-0.6734E-04	0.1381E-03	0.3303E-03	0.5396E-04	-0.1627E-02	0.9323E-03
24.130	-0.7639E-04	0.1391E-03	0.3327E-03	0.5437E-04	-0.1639E-02	0.9393E-03
25.350	-0.6149E-04	0.1402E-03	0.3351E-03	0.5479E-04	-0.1651E-02	0.9462E-03
26.620	-0.6609E-04	0.1412E-03	0.3375E-03	0.5520E-04	-0.1663E-02	0.9530E-03
27.930	-0.6257E-04	0.1422E-03	0.3398E-03	0.5561E-04	-0.1675E-02	0.9598E-03
29.300	-0.5704E-04	0.1432E-03	0.3421E-03	0.5602E-04	-0.1686E-02	0.9665E-03
30.710	-0.5783E-04	0.1442E-03	0.3444E-03	0.5644E-04	-0.1698E-02	0.9732E-03
32.180	-0.4686E-04	0.1452E-03	0.3467E-03	0.5685E-04	-0.1709E-02	0.9799E-03
33.710	-0.5101E-04	0.1462E-03	0.3490E-03	0.5727E-04	-0.1721E-02	0.9865E-03

Figure 6-15. Part of File *co2d_min.dat* for Problem No. 5, Giving Changes in Mineral Abundances (Volume Fraction) after t = 10 yr. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

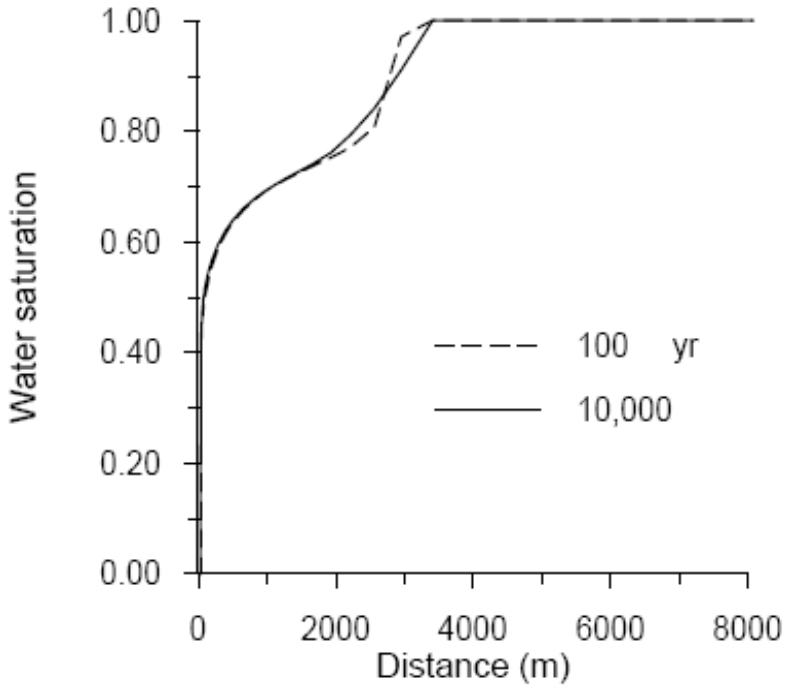

Figure 6-16. Water Saturations at Different Times for the One-Dimensional Radial Flow Problem. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

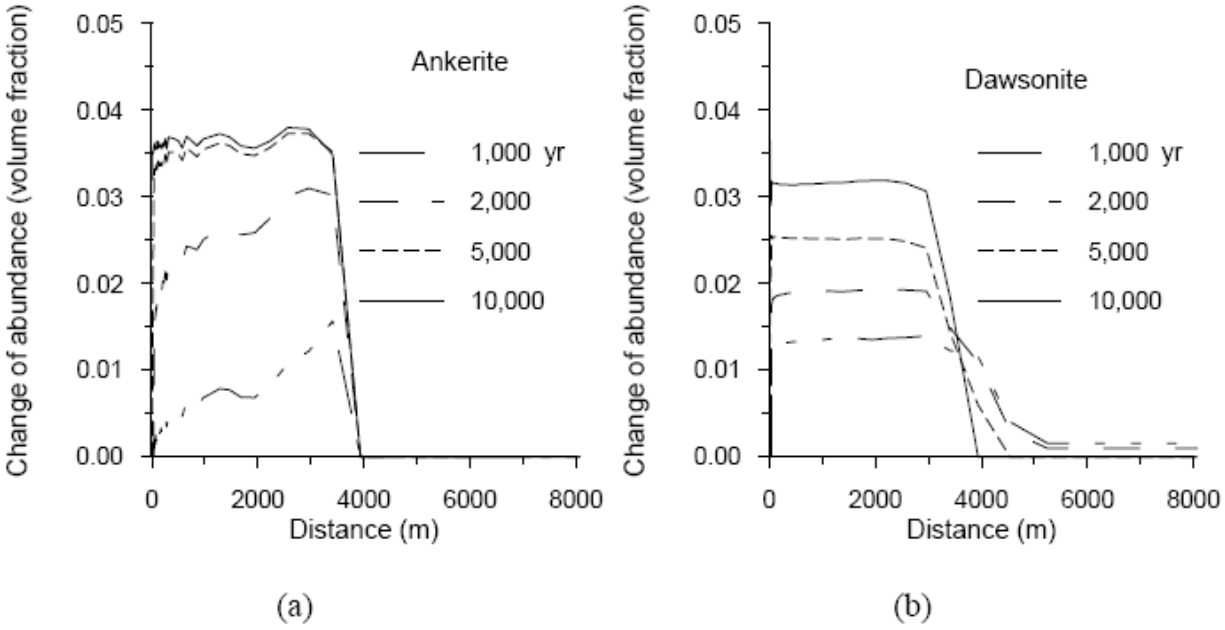

Figure 6-17. Change in Mineral Abundance (Negative Values Indicate Dissolution and Positive Precipitation) after Different Times for the One-Dimensional Radial Flow Problem. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

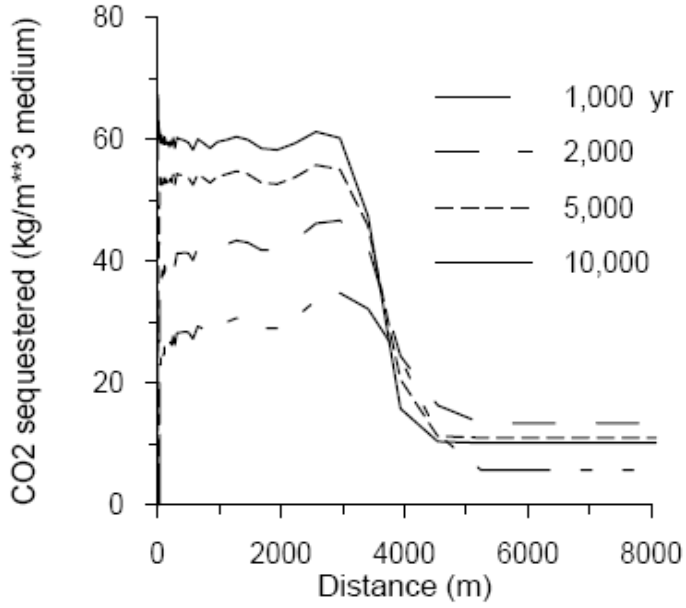

Figure 6-18. Cumulative CO_2 Sequestration by Carbonate Precipitation for Different Times. The Positive Values in the Background Region (x > 4000 m) are Due to Calcite Precipitation. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

With the exception of calculation time from *flow.out*, the output files for this problem are identical to the files that accompany the program. Parts of the output files for fluid flow, aqueous chemical concentrations, and changes of mineral abundances are given in Figures 6-19, 6-20, and 6-21. These tables correlate to the graphical representations of water saturation, change in mineral abundance, and pH and dissolved Cu^{2+} concentration versus distance and depth (Figures 6-22, 6-23, 6-24).

6.3.7 Caprock Alteration—Module EOS2

This problem simulates the interaction between hydrothermal fluids and geomedia as the fluid migrates from the thermal source toward the surface (Xu and Pruess, 2001). The problem is based on the Long Valley Caldera, California (Sorey, 1985; White and Peterson, 1991; Sorey, et al., 1998). The flow system is simplified to a single vertical fracture domain and a matrix domain that is discretized into six grid zones with permeability decrease as a function of distance from the fracture. The objective of this simulation is to demonstrate the proper handling of the following processes:

- Fracture-matrix interaction (fluid, heat, and chemical species)
- Gas phase contribution to multiphase flow and chemical reactions
- Kinetic chemical reactions
- Effect of heat on chemical properties and geochemical processes

This simulation provides predictions of water saturation, heat distribution, and change in mineral abundances as a function of depth and distance from the fracture.

With the exception of calculation time from *flow.out*, the output files for this problem are identical to the files that accompany the program. Contour plots of steady-state liquid water saturation and temperature are presented in Figure 6-25. Some results for changes of mineral abundances are given in Figures 6-26 and 6-27. More results can be found in Xu and Pruess (2001a).

6.3.8 Injection Well Scaling and Acidizing at Tiwi Field, Philippines—Module EOS1

This one-dimensional radial flow problem simulates the injection of a hot brine solution into a fractured porous media. High silica concentrations in the brine lead to scaling in the well bore and loss of injection capacity. The objective of this simulation is to demonstrate the proper handling of heat transfer between brine and the formation, precipitation of silica on the well bore, and the dissolution of silica by injection of acid. This simulation compares the loss of injection capacity with the measured values over a 12-year period. In addition, predictions of the amount of amorphorous silica precipitated and changes in fractured permeability and matrix permeability as a function of distance from the well bore are presented. Additional results are presented by Xu, et al. (2004).

```
     4( 1, 1) ST = 0.100000E+02 DT = 0.100000E+02 DX1= 0.000000E+00
     4( 2, 1) ST = 0.300000E+02 DT = 0.200000E+02 DX1= 0.000000E+00
     4( 3, 1) ST = 0.500000E+02 DT = 0.200000E+02 DX1= 0.000000E+00
     4( 4, 1) ST = 0.700000E+02 DT = 0.200000E+02 DX1= 0.000000E+00
     4( 5, 1) ST = 0.900000E+02 DT = 0.200000E+02 DX1= 0.000000E+00
     4( 6, 1) ST = 0.110000E+03 DT = 0.200000E+02 DX1= 0.000000E+00
     4( 7, 1) ST = 0.130000E+03 DT = 0.200000E+02 DX1= 0.000000E+00
     4( 8, 1) ST = 0.150000E+03 DT = 0.200000E+02 DX1= 0.000000E+00
     4( 9, 1) ST = 0.190000E+03 DT = 0.400000E+02 DX1= 0.000000E+00
     4( 10, 1) ST = 0.270000E+03 DT = 0.800000E+02 DX1= 0.000000E+00
     4( 11, 1) ST = 0.430000E+03 DT = 0.160000E+03 DX1= 0.000000E+00
     4( 12, 1) ST = 0.750000E+03 DT = 0.320000E+03 DX1= 0.000000E+00
     4( 13, 1) ST = 0.139000E+04 DT = 0.640000E+03 DX1= 0.000000E+00
     4( 14, 2) ST = 0.267000E+04 DT = 0.128000E+04 DX1= -.492268E-07
     4( 15, 2) ST = 0.523000E+04 DT = 0.256000E+04 DX1= -.983198E-07
     4( 16, 2) ST = 0.103500E+05 DT = 0.512000E+04 DX1= -.196049E-06
OUTPUT DATA AFTER ( 752, 1)-2-TIME STEPS
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TOTAL TIME KCYC ITER ITERC KON DX1M
0.31558E+09 752 1 1004 2 0.00000E+00
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
    ELEM. INDEX PRES S(liq) PCAP K(rel) DIFFUS.
    (PA) (PA) (m^2/s)
    1 1 0.10000E+06 0.26920E+00 -.28545E+05 0.14549E-04 0.43643E-08
    2 1 2 0.10000E+06 0.97604E+00 -.44650E+05 0.51412E+00 0.75893E-06
    3 1 3 0.10000E+06 0.97604E+00 -.44652E+05 0.51411E+00 0.75890E-06
    4 1 4 0.10000E+06 0.97603E+00 -.44655E+05 0.51409E+00 0.75882E-06
    5 1 5 0.10000E+06 0.97603E+00 -.44662E+05 0.51404E+00 0.75866E-06
    6 1 6 0.10000E+06 0.97601E+00 -.44674E+05 0.51395E+00 0.75838E-06
    7 1 7 0.10000E+06 0.97600E+00 -.44687E+05 0.51385E+00 0.75809E-06
    2 8 0.10000E+06 0.25773E+00 -.30149E+05 0.88699E-05 0.29194E-08
```

Figure 6-19. Part of File *flow.out* for Problem No. 6 (Copper Enrichment). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

X	Y	Sl	pH	so4-2	fe+2	cu+2	na+
0.000	-1.000	0.2692	3.2654	0.1423E-02	0.5471E-08	0.2369E-03	0.4477E-03
0.254	-1.000	0.9760	3.2604	0.1439E-02	0.5632E-08	0.2396E-03	0.4528E-03
0.900	-1.000	0.9760	3.2491	0.1503E-02	0.5869E-08	0.2502E-03	0.4724E-03
2.247	-1.000	0.9760	3.2277	0.1637E-02	0.6361E-08	0.2725E-03	0.5136E-03
5.215	-1.000	0.9760	3.1916	0.1905E-02	0.7343E-08	0.3170E-03	0.5957E-03
10.790	-1.000	0.9760	3.1492	0.2341E-02	0.8840E-08	0.3897E-03	0.7300E-03
14.340	-1.000	0.9760	3.1295	0.2776E-02	0.9809E-08	0.4631E-03	0.8657E-03
0.000	-3.000	0.2577	3.1261	0.2571E-02	0.9693E-08	0.3357E-03	0.8379E-03
0.254	-3.000	0.9832	3.1257	0.2577E-02	0.9825E-08	0.3365E-03	0.8401E-03
0.900	-3.000	0.9832	3.1235	0.2596E-02	0.9924E-08	0.3379E-03	0.8465E-03
2.247	-3.000	0.9832	3.1173	0.2635E-02	0.1020E-07	0.3392E-03	0.8602E-03
5.215	-3.000	0.9832	3.0930	0.2707E-02	0.1132E-07	0.3342E-03	0.8881E-03
10.790	-3.000	0.9832	3.0012	0.2789E-02	0.1736E-07	0.2813E-03	0.9364E-03
14.340	-3.000	0.9832	3.1751	0.2676E-02	0.6674E-03	0.1940E-12	0.9870E-03

Figure 6-20. Part of File *Amic_aqu.dat* for Problem No. 6 after t = 10 yr (Sl is Water Saturation, Unit of Concentrations is mol/l). Figure from Xu et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

X	Y	pyrite	chalcopyrit	magnetite	k-feldspar	albite
0.000	-1.000	-0.1611E-06	-0.1441E-06	-0.7489E-07	-0.1135E-07	-0.6221E-06
0.254	-1.000	-0.2149E-05	-0.1922E-05	-0.9993E-06	-0.1515E-06	-0.8300E-05
0.900	-1.000	-0.2149E-05	-0.1922E-05	-0.9993E-06	-0.1515E-06	-0.8300E-05
2.247	-1.000	-0.2149E-05	-0.1922E-05	-0.9993E-06	-0.1515E-06	-0.8300E-05
5.215	-1.000	-0.2149E-05	-0.1922E-05	-0.9992E-06	-0.1515E-06	-0.8299E-05
10.790	-1.000	-0.2149E-05	-0.1922E-05	-0.9992E-06	-0.1515E-06	-0.8299E-05
14.340	-1.000	-0.2149E-05	-0.1922E-05	-0.9992E-06	-0.1515E-06	-0.8299E-05
0.000	-3.000	-0.1542E-06	-0.1380E-06	-0.7170E-07	-0.1087E-07	-0.5956E-06
0.254	-3.000	-0.2165E-05	-0.1937E-05	-0.1007E-05	-0.1526E-06	-0.8360E-05
0.900	-3.000	-0.2165E-05	-0.1937E-05	-0.1007E-05	-0.1526E-06	-0.8360E-05
2.247	-3.000	-0.2165E-05	-0.1937E-05	-0.1007E-05	-0.1526E-06	-0.8360E-05
5.215	-3.000	-0.2165E-05	-0.1937E-05	-0.1007E-05	-0.1526E-06	-0.8360E-05
10.790	-3.000	-0.2165E-05	-0.1937E-05	-0.1007E-05	-0.1526E-06	-0.8360E-05
14.340	-3.000	-0.1920E-05	-0.1912E-05	-0.1007E-05	-0.1526E-06	-0.8360E-05

Figure 6-21. Part of File *Amic_sod.dat* for Problem No. 6, Giving Changes in Mineral Abundances (in Volume Fraction, Positive Values Indicate Precipitation and Negative Dissolution) After t = 10 yr. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output are Shown as One Set of Identical Data.

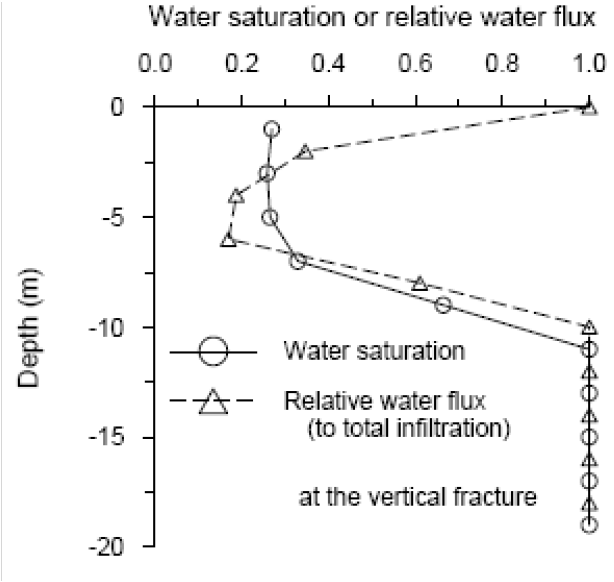

Figure 6-22. Steady-State Water Saturation and Water Flux (Relative to Total Infiltration) Passed Through the Fractures. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

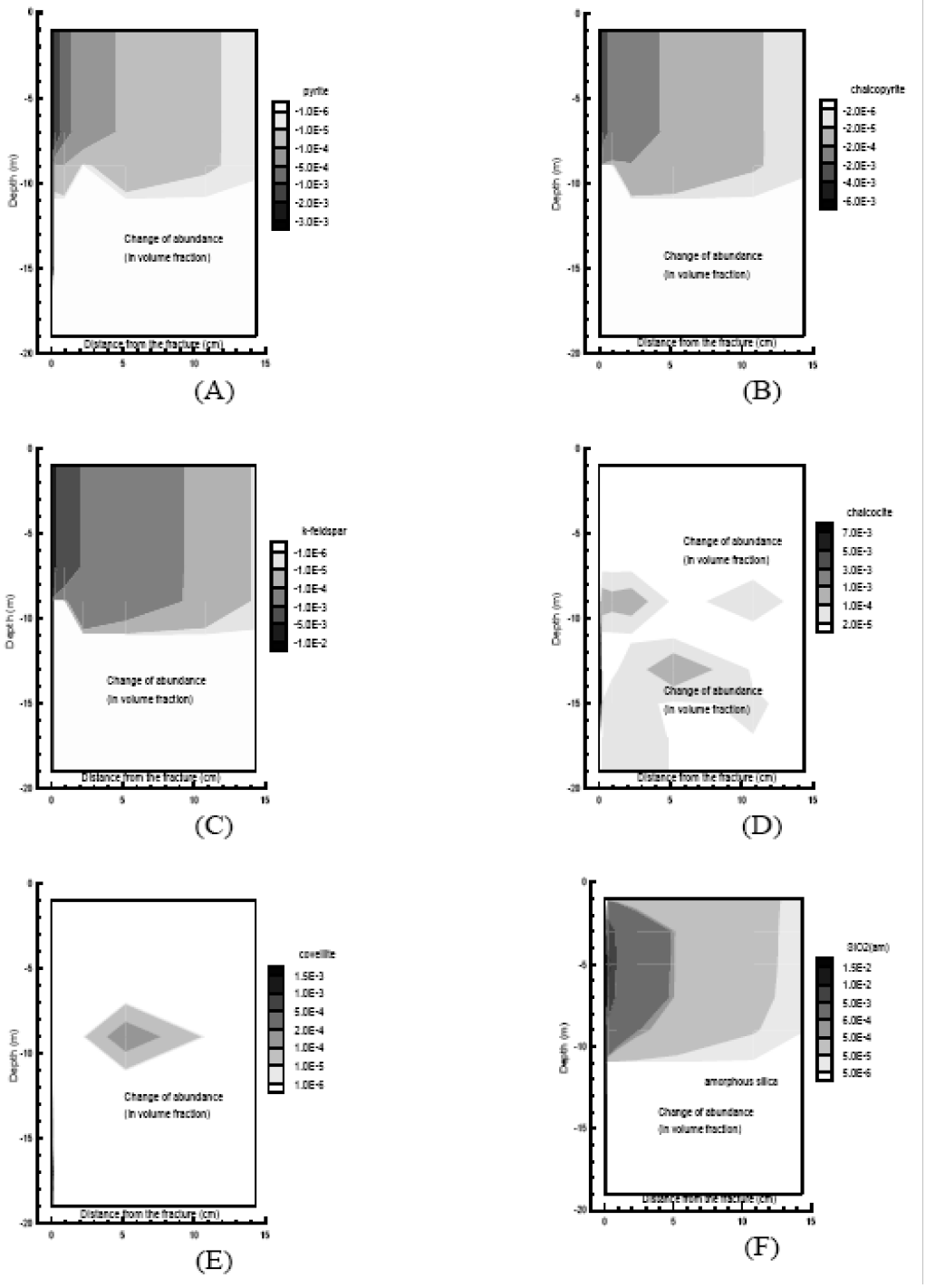

Figure 6-23. Change of Mineral Abundance (Positive Values Indicate Precipitation and Negative Dissolution) after 20,000 Yrs in the Fractured Rock. Figure from Xu, et Al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

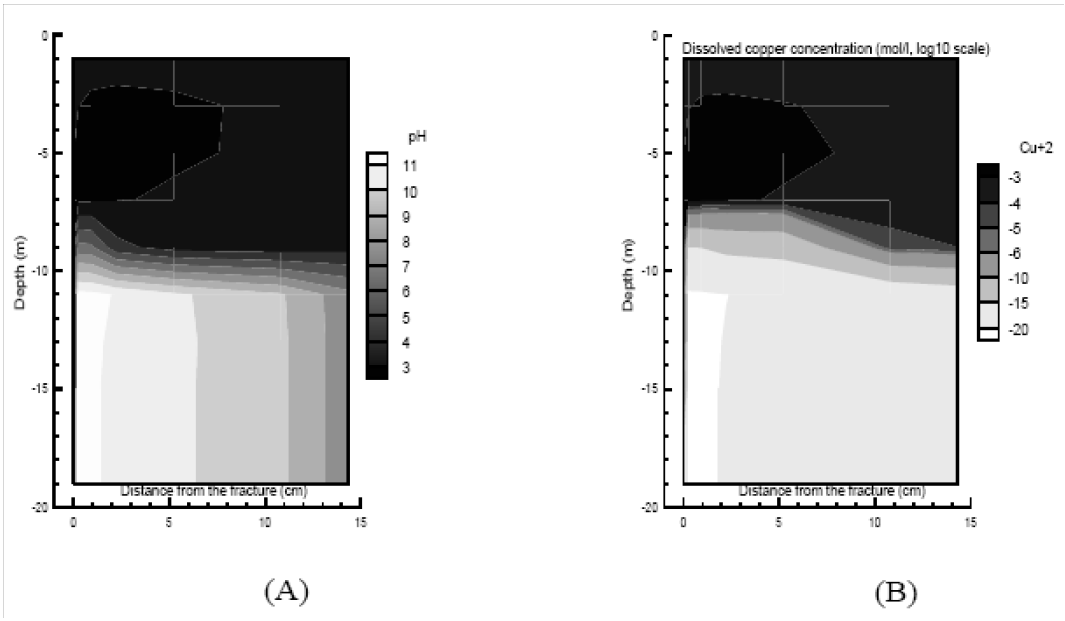

Figure 6-24. pH and Dissolved Copper Concentration at 20,000 Yrs in the Fractured Rock. Figure from Xu, et Al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

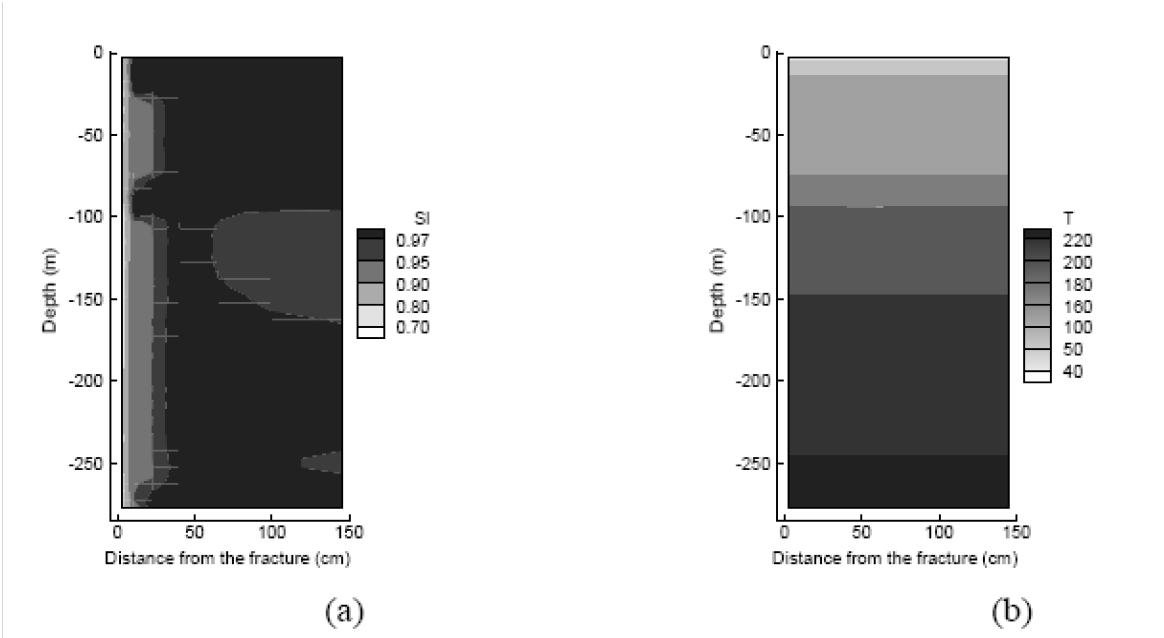

Figure 6-25. Liquid Saturation (a) and Temperature (b, in ˚C) in the Fracture-matrix System. This and Subsequent Contour Plots Extend to a Distance of 145 cm [57.09 in], Which Is the Distance Between the Center of the Fracture Zone, and the Nodal Point at the Center of the Innermost Matrix Grid Block. The Overall Size of the Model Domain is 175 cm [68.9 in]. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

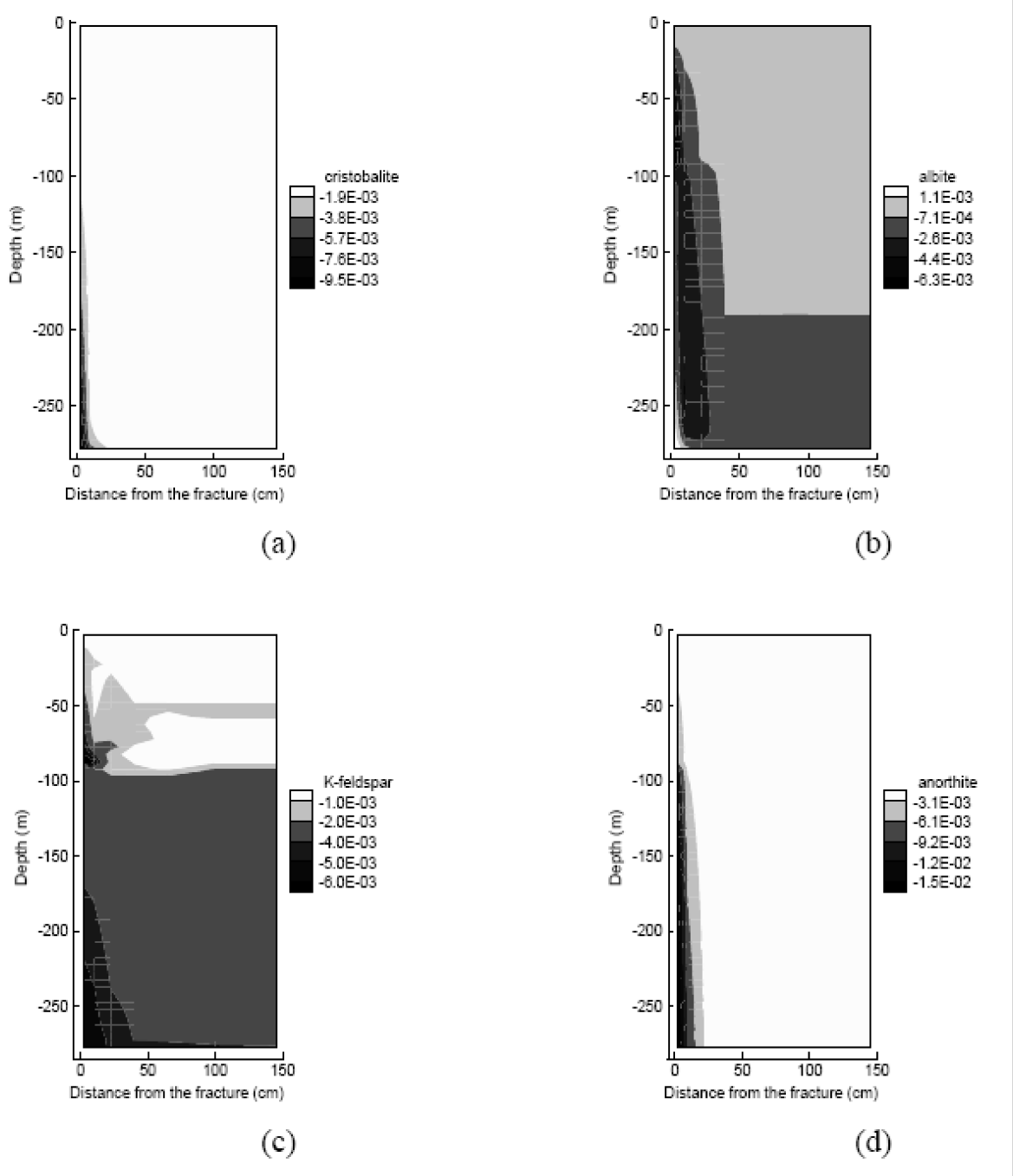

Figure 6-26. Change of Primary Mineral Abundance (In Volume Fraction) after 1,000 years. The Inflection Points in the Figures Result from (i) Grid Discretization and (Ii) Highly Non-Linear Nature of Heterogeneous Reactions. The Space Discretization in the Simulation Is Not Fine Enough to Give an Accurate Definition of Mineral Abundances near Inflection Points. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

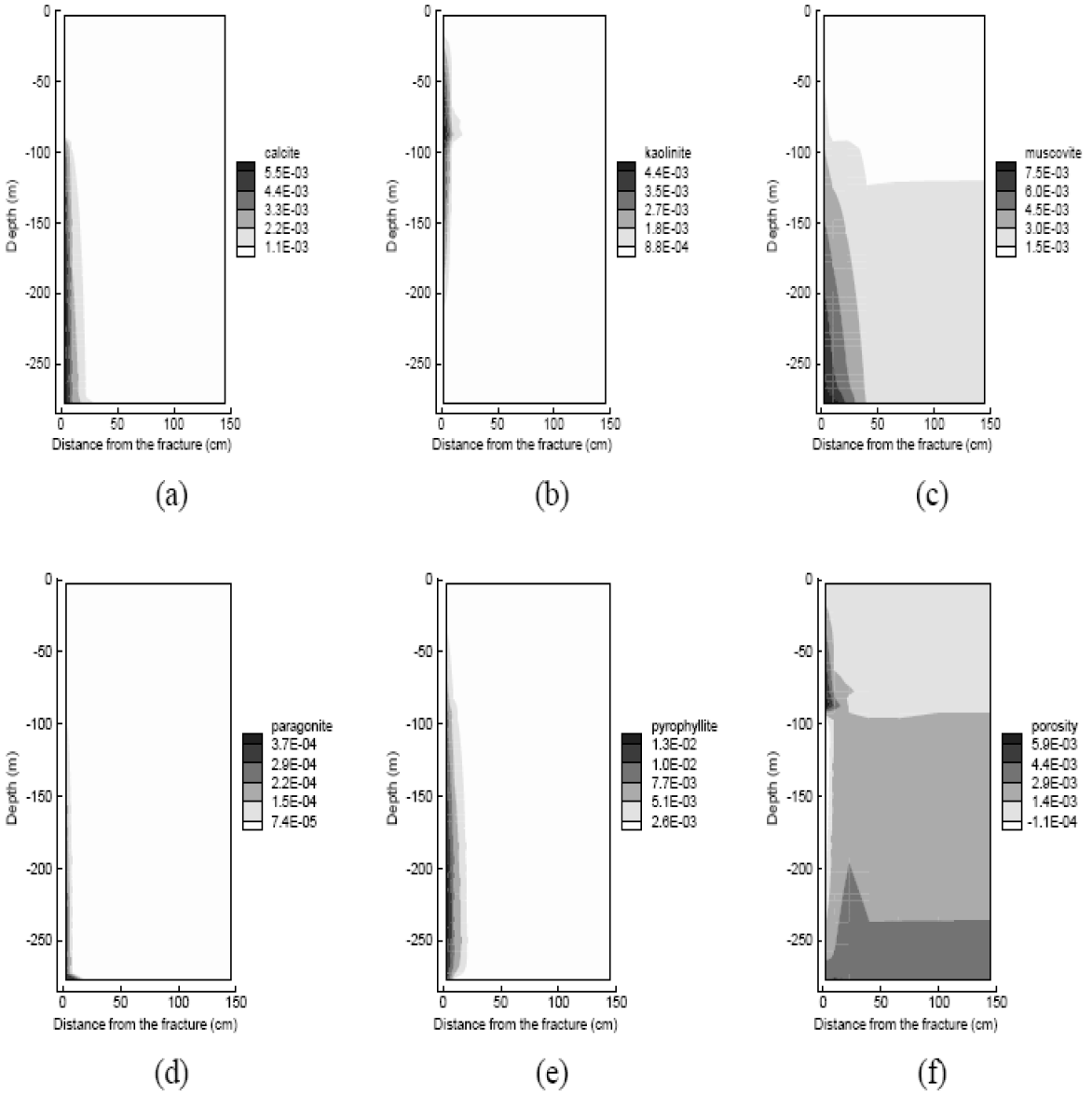

Figure 6-27. Change of Mineral Abundance (Secondary Phases, in Volume Fraction) and Porosity after 1,000 Years. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

With the exception of calculation time from *flow.out*, the output files for this problem are identical to the files that accompany the program. Parts of the output files for fluid flow, aqueous chemical concentrations, and changes of mineral abundances are given in Figures 6-28, 6-29, and 6-30.

One of the hot brine injectors located to the southeast of the Tiwi geothermal field, Philippines had a significant decrease in injectivity with time. The drop in injection capacity was attributed to scaling inside the wellbore, which was mostly attributed to amorphous silica precipitation. Using historical chemical records, the degree of amorphous silica saturation in each analyzed water sample was determined. Modeling the amorphous silica injection rates was used to identify factors that cause the deposition of amorphous silica in the near-well formation and the extent of their effect using TOUGHREACT. These factors include the silica concentration in the hot brine injectate, the temperature of the injectate, the flowrate of the injectate, the pH of the injectate, and the temperature and pressure conditions of the reservoir in the vicinity of the injector. Based on the silica injection index (Figure 6-31), it was determined that significant reductions in porosity and permeability occur within a 10 m [32.81 ft] radius of the well (Figure 6-32). The porosity reduction is mainly due to precipitation of amorphous silica (Figure 6-33). Some low-albite precipitation and minor illite precipitation and calcite dissolution occur in the simulations.

```
A1 5( 1, 4) ST = 0.262800E+07 DT = 0.100000E+01 DX1= 0.191361E+06 DX2= -.307680E+01
A1 4( 2, 3) ST = 0.262800E+07 DT = 0.100000E+01 DX1= 0.281361E+05 DX2= -.164174E+02
A1 4( 3, 3) ST = 0.262800E+07 DT = 0.100000E+01 DX1= 0.147272E+05 DX2= -.128794E+02
A1 4( 4, 3) ST = 0.262800E+07 DT = 0.100000E+01 DX1= 0.101133E+05 DX2= -.101427E+02
A1 4( 5, 3) ST = 0.262800E+07 DT = 0.100000E+01 DX1= 0.778018E+04 DX2= -.801140E+01
---------------------------
OUTPUT DATA AFTER (1469, 3)-2-TIME STEPS
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
TOTAL TIME KCYC ITER ITERC KON DX1M DX2M DX3M
0.31558E+08 1469 3 4299 2 0.206859E+06 0.289189E-01 0.000000E+00
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
ELEM. INDEX P T SG SW X1 X2
(PA) (DEG-C)
A1 3 1 0.12355E+08 0.16041E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00
A1 4 2 0.12327E+08 0.16041E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00
A1 5 3 0.12302E+08 0.16042E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00
A1 6 4 0.12277E+08 0.16042E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00
A1 7 5 0.12254E+08 0.16042E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00
```

Figure 6-28. Part of File *flow.out* for Problem No. 8 (Injection Well Scaling). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

X	T	pH	ca+2	mg+2	na+	sio2(aq)	hco3-
0.139	160.408	6.7397	0.1033E-02	0.1729E-04	0.1273E+00	0.1164E-01	0.1042E-02
0.179	160.412	6.7397	0.1033E-02	0.1730E-04	0.1273E+00	0.1164E-01	0.1042E-02
0.228	160.416	6.7397	0.1033E-02	0.1731E-04	0.1273E+00	0.1164E-01	0.1042E-02
0.286	160.419	6.7398	0.1033E-02	0.1733E-04	0.1273E+00	0.1164E-01	0.1042E-02
0.356	160.422	6.7398	0.1033E-02	0.1735E-04	0.1273E+00	0.1164E-01	0.1042E-02
0.440	160.425	6.7398	0.1033E-02	0.1738E-04	0.1273E+00	0.1164E-01	0.1042E-02
0.539	160.429	6.7399	0.1033E-02	0.1743E-04	0.1273E+00	0.1164E-01	0.1043E-02
0.658	160.432	6.7400	0.1033E-02	0.1750E-04	0.1273E+00	0.1164E-01	0.1043E-02
0.801	160.435	6.7401	0.1033E-02	0.1759E-04	0.1273E+00	0.1164E-01	0.1043E-02
0.971	160.437	6.7403	0.1033E-02	0.1773E-04	0.1273E+00	0.1164E-01	0.1043E-02
1.174	160.440	6.7406	0.1033E-02	0.1792E-04	0.1273E+00	0.1164E-01	0.1043E-02
1.417	160.444	6.7410	0.1033E-02	0.1820E-04	0.1273E+00	0.1164E-01	0.1043E-02
1.708	160.447	6.7416	0.1033E-02	0.1860E-04	0.1273E+00	0.1164E-01	0.1043E-02
2.056	160.450	6.7423	0.1033E-02	0.1915E-04	0.1273E+00	0.1164E-01	0.1043E-02
2.471	160.454	6.7434	0.1033E-02	0.1993E-04	0.1273E+00	0.1164E-01	0.1043E-02
2.967	160.459	6.7449	0.1033E-02	0.2099E-04	0.1273E+00	0.1165E-01	0.1043E-02
3.561	160.465	6.7469	0.1033E-02	0.2241E-04	0.1273E+00	0.1165E-01	0.1043E-02
4.271	160.472	6.7495	0.1033E-02	0.2426E-04	0.1273E+00	0.1165E-01	0.1043E-02

Figure 6-29. Part of File *sca_conc.dat* for Problem No. 8 After t = 1 yr (T is Temperature in ºC, Unit of Concentrations is mol/l). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

X	Porosity	Permeability	calcite	albite-low	illite	sio2(amor.)
0.139	0.49861	0.30213E-11	-0.1660E-04	0.7874E-03	0.9664E-04	0.1337E-02
0.179	0.49862	0.30304E-11	-0.1660E-04	0.7875E-03	0.9662E-04	0.1326E-02
0.228	0.49864	0.30387E-11	-0.1660E-04	0.7875E-03	0.9660E-04	0.1315E-02
0.286	0.49865	0.30470E-11	-0.1660E-04	0.7876E-03	0.9658E-04	0.1304E-02
0.356	0.49866	0.30544E-11	-0.1660E-04	0.7876E-03	0.9656E-04	0.1295E-02
0.440	0.49867	0.30627E-11	-0.1660E-04	0.7876E-03	0.9653E-04	0.1284E-02
0.539	0.49868	0.30712E-11	-0.1660E-04	0.7875E-03	0.9649E-04	0.1274E-02
0.658	0.49869	0.30791E-11	-0.1660E-04	0.7874E-03	0.9643E-04	0.1264E-02
0.801	0.49870	0.30886E-11	-0.1660E-04	0.7872E-03	0.9635E-04	0.1252E-02
0.971	0.49871	0.30979E-11	-0.1659E-04	0.7869E-03	0.9625E-04	0.1240E-02
1.174	0.49872	0.31097E-11	-0.1659E-04	0.7864E-03	0.9610E-04	0.1226E-02
1.417	0.49874	0.31234E-11	-0.1659E-04	0.7856E-03	0.9589E-04	0.1209E-02
1.708	0.49876	0.31389E-11	-0.1658E-04	0.7845E-03	0.9558E-04	0.1190E-02
2.056	0.49879	0.31594E-11	-0.1657E-04	0.7829E-03	0.9516E-04	0.1165E-02
2.471	0.49882	0.31846E-11	-0.1656E-04	0.7806E-03	0.9454E-04	0.1134E-02
2.967	0.49886	0.32188E-11	-0.1654E-04	0.7772E-03	0.9366E-04	0.1093E-02
3.561	0.49891	0.32634E-11	-0.1652E-04	0.7722E-03	0.9240E-04	0.1040E-02
4.271	0.49898	0.33240E-11	-0.1648E-04	0.7651E-03	0.9058E-04	0.9683E-03

Figure 6-30. Part of File *sca_min.dat* for Problem No. 8 After t = 1 yr (Unit of Permeability is m^2; Mineral Abundances are Expressed as Changes in Volume Fraction, Positive Values Indicate Precipitation and Negative Dissolution). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical data.

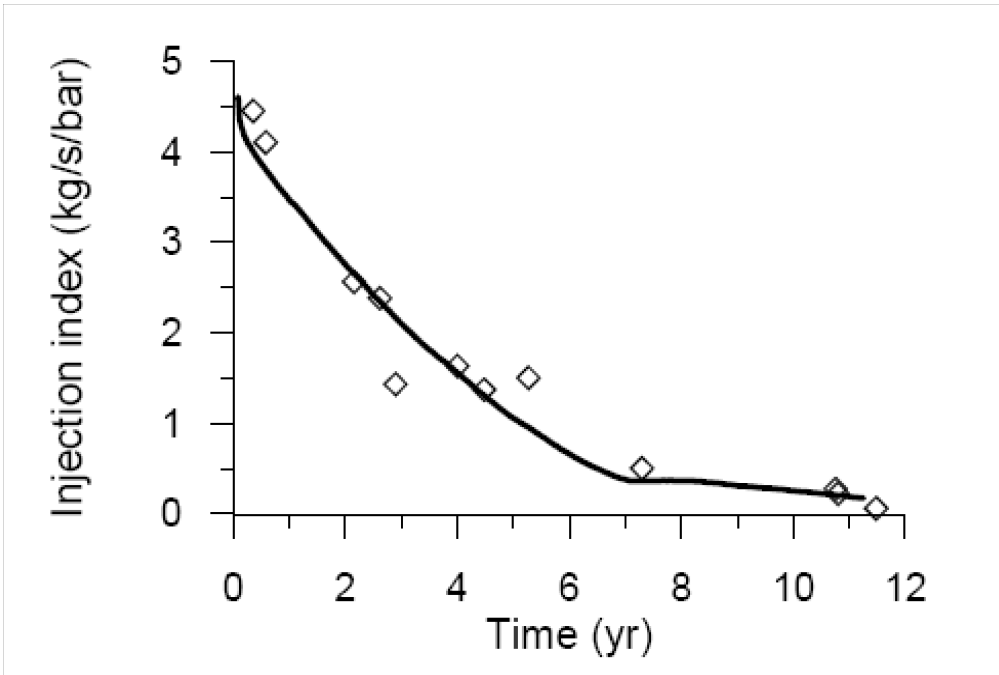

Figure 6-31. Simulated Injection Indexes Using an Injection Temperature of 161 °C [322 °F] for the Later Time Period, Together with Measured Data (Silica Concentration = 705 ppm, ϕ_c = 0.92%, and n = 10). Figure from Xu, et al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

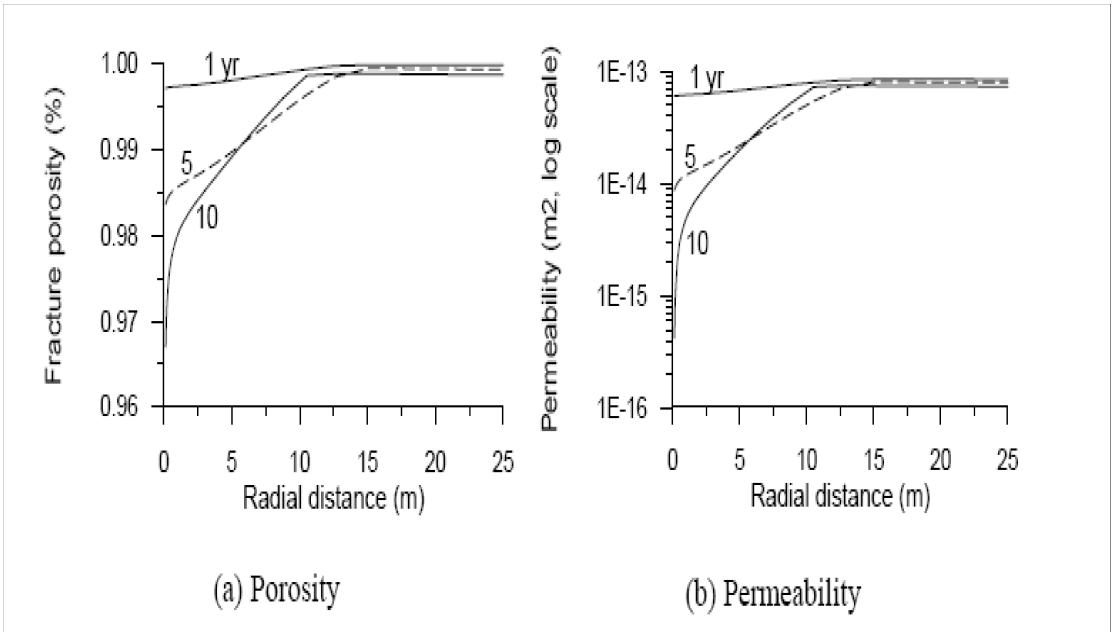

Figure 6-32. Distribution of Porosity and Permeability along the Well Radius for the Simulation Shown in Figure 6.3.8.4. Figure from Xu, et al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

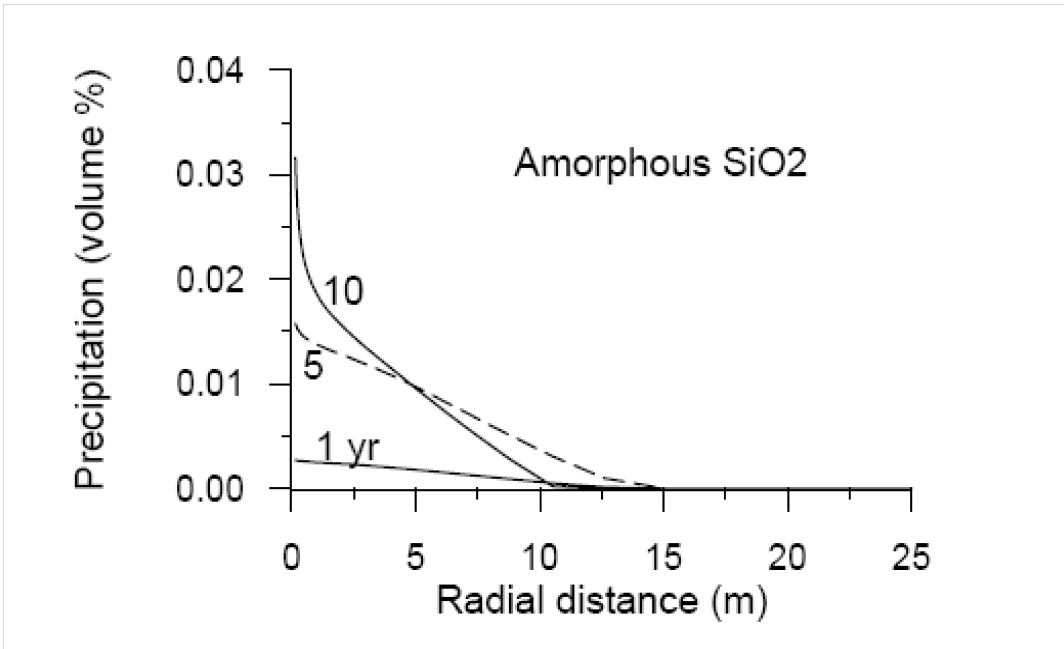

Figure 6-33. Amorphous Silica Precipitated Along the Well Radius for the Simulation Shown in Figure 6.3.8.4. Figure from Xu, et Al., 2005. Results for the Validation and Supplied Output Are Shown as One Set of Identical Data.

APPENDIX A

CONTENTS OF README.TXT FILE

```
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$                                                                                    $
$                                                                                    $
$     *************************************************************************      $
$     *******************  TOUGHREACT  October 2004    ************************      $
$     *************************************************************************      $
$                                                                                    $
$     .......READ.ME..........READ.ME..........READ.ME..........READ.ME........      $
$     .........................................................................      $
$     .............................Update 10/04................................      $
$     .........................................................................      $
$                                                                                    $
$                                                                                    $
$        TOUGHREACT is a program for non-isothermal multiphase reactive fluid        $
$     flow and geochemical transport in porous media and fractured rocks. The code   $
$     is written in Fortran 77. It is developed by introducing reactive geochemical  $
$     transport into the framework of the existing multi-phase fluid and heat        $
$     flow code TOUGH2 V2 (Pruess et al., 1999).                                     $
$                                                                                    $
$                 Developed by                                                       $
$                             Tianfu Xu                                              $
$                             Eric Sonnenthal                                        $
$                             Nicolas Spycher                                        $
$                             Karsten Pruess                                         $
$                                                                                    $
$                           At Lawrence Berkeley National Laboratory                 $
$                                                                                    $
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
```

This flyer contains brief instructions for installing and running TOUGHREACT

TOUGHREACT is distributed on CD. Because TOUGHREACT was derived from TOUGH2 V2,in addition to the current manual, users must have the manual of the TOUGH2 V2 (Pruess et al., 1999). Information on TOUGH2 V2 is also available on the TOUGH2 homepage on the web.

```
**************************************************************************
*                 http://www-esd.lbl.gov/TOUGH2/                         *
**************************************************************************
```

==========

1. THIS CD INCLUDES FIVE SUBDIRECTORIES:

1.1. Subdirectory: 'documents' contains the manual of the TOUGHREACT code.

1.2. Subdirectory: 'source-files' contains source files of the code:

```
   treact.f       - This module contains the main program of TOUGHREACT, and
                    must be compiled with INCLUDE files 'T2', 'chempar23.inc',
                    common23.inc, and 'perm23.inc' with PARAMETER statements
                    for flexible dimensioning of all major arrays;

   T2             - an INCLUDE file for PARAMETER statements of fluid and
                    heat flow;
```

chempar23.inc - an INCLUDE file for PARAMETER statements of reactive geochemical transport;

common23.inc - an INCLUDE file for common blocks for reactive geochemical transport;

perm23.inc - an INCLUDE file for PARAMETER statements related to porosity and permeability changes due to mineral dissolution and precipitation;

t2cg22.f - includes an executive routine LINEQ for the linear equation solution, which may call a solver package t2solv.f. It also includes routines for preconditioning of the Jacobian matrix;

t2solv.f - a package of conjugate gradient solvers;

meshm.f - module with internal mesh generation facilities;

t2f.f - the core module of TOUGH2; it reads input data, initializes arrays and parameters, sets up the Jacobian matrix for Newton-Raphson iteration, and performs time stepping. It also contains the water property routines (steam table equations) and the relative permeability and capillary pressure functions which are used in the equation-of-state modules;

multi.f - formulate Jacobian matrix and right-hand side residual terms for multi-phase fluid and heat flow;

readsolu.f - read and initialize data related to solute transport;

inichm.f - read and initialize data related to geochemistry;

geochem.f - subroutines for geochemical calculations and writing aqueous concentrations and mineral abundances at specified time steps;

newton.f - assemble Jacobian matrix of Newton-Raphson iteration for solving equations of geochemical system;

rctprop.f - calculate (1) reactive surface areas for reactions of mineral dissolution and precipitation, (2) porosity and permeability changes due to mineral dissolution and precipitation, and (3) Leverett scaling for capillary pressure modification due to porosity and permeability changes;

ma28abc.f - MA28 linear equation solver is not available for TOUGHREACT unlike TOUGH2. TOUGHREACT uses only onjugate gradient(iterative) solvers. To avoid unsatisfied externals, some dummy subroutines are placed in file ma28abc.f.

Two versions of the TOUGHREACT source program are available on the distribution CD. One contains IMPLICIT DOUBLE PRECISION (A-H, O-Z) and IMPLICIT INTEGER*8 (I-N) statements that will automatically generate 64-bit arithmetic on 32 bit processors. Another contains the same code but without the INTEGER*8 statements, because most PC compilers do not recognize the *8 statements. The latter version may require special compliler options to generate 64-bit code at compile time. Therefore, two subdirectories: 'integerx8' and 'integer', are created coresponding to the two versions. Note that the original TOUGH2 V2.0 is intrinsically single-precision and requires special compliler options to generate 64-bit code at compile time.

Each version also includes three low-level subdirectories: (1) 'EOS-modules' (equation of state for fluid flow, see original TOUGH2 V2 manual; Pruess et al.,1999), (2) 'SECOND-subroutines' (CPU-time subroutine that is machine-dependent), and (3) 'makefiles' (used for compiling and linking, which is compiler-dependent).

'EOS-modules' contains:

eos1.f - equation of state for water, or two waters;
eos2.f - equation of state for water/CO2 mixtures;
eos3.f - equation of state for water/air;
eos4.f - equation of state for water/air (with vapor pressure lowering effects);
eos9.f - equation of state for saturated-unsaturated flow (Richards' equation);
eco2.f - equation of state for water-brine-CO2 mixtures (for CO2 deep saline aquifer disposal). This routine requires a property data file CO2TAB is required, which can be found in the current subdirectory.

'SECOND-subroutines' contains:

second_pc.f - timer subroutine for PC
second_mac.f - timer subroutine for Macintosh
second_sun.f - timer subroutine for SUN workstation
second_dec.f - timer subroutine for DEC ALPHA workstation
second_ibm.f - timer subroutine for IBM RISC System/6000 workstation, running a UNIX-based operating system

'makefile':

makefile for DEC ALPHA Workstation, or
SUN SPARC Workstation, or
Intel Fortran Compiler on linux, or
Mac PPC - g77, or
IBM - f77

1.3. Subdirectory: 'sample-problems'

The directory contains a total of 8 subdirectories. Each subdirectory contains one sample problem. Simulations of sample problem presented here were run on Pentium 4 PC machines (1.7G). These EXE files were generated with COMPAQ Visual Fortran compiler version 6.6, and are also provided in the distribution CD. The descriptions of sample problems are given in Chapter 8 of the manual.

'P1_EOS9_kd-decay': Linear sorption and decay.

'P2_EOS9_Aquia-aquifer': Water quality in the Aquia aquifer.

'P3_EOS3_YM-calcite': Infiltration and calcite deposition at Yucca Mountain.

'P4_EOS4_Heat-test': Yucca Mountain heat test problem.

'P5_ECO2_1D-radial': CO2 disposal in deep aquifers.

'P6_EOS9_copper': Supergene copper enrichment.

'P7_EOS2_LVC': Caprock alteration in Long Valley Cadera (LVC).

'P8_EOS1_scaling': Reservoir mineral scaling by injection.

1.4. Subdirectory: 'EXE-files-PC'

This contains executable files with different fluid flow modules for running problems on PCs. The PC EXE files were generated with COMPAQ Visual Fortran compiler 6.6.

1.5. Subdirectory: 'utility-programs'

The 'utility-programs' directory provides utility programs for the chemical database. The descriptions of these programs are given in Appendix J of the TOUGHREACT manual. It includes four low-level subdirectories:

'convert-eq3/6' contains the source code and an example input for converting EQ3/6 database (data0) to TOUGHREACT database.

'switch-basis' contains the source code and an example input for switching basis (primary) species.

'regress-logK' contains the source code for regressing logK data.

'check-balance' contains the source code and an example input for checking mass and charge balances of reactions.

==========

2. CODE INSTALLATION

Step 1: Create a directory in user's computer

Step 2: Copy all files from the root of subdirectory 'source-files/integerx8'

Step 3: If necessary, adjust parameter statements (dimensioning variables)
in T2 (for fluid and heat flow dimension parameters) and
chempar23.inc file (for chemistry dimension parameters)
to be sufficient for the simulation problem.
For example, MNEL = 8000 (maximum number of grid blocks)
and MNCON = 20000 (maximum number of connections) are specified
in the INCLUDE file T2 with the distribution CD.

Step 4: Copy a desired EOS-module from the low-level subdirectory
'EOS-modules'. Note that only one of the EOS modules must
be linked at a time.

Step 5: Copy a timer subroutine from the low-level subdirectory
'SECOND-subroutines', depending on user's machine.

Step 6: Copy makefile from the low-level subdirectory 'makefile', and modify
the provided makefile depending on user's machine and compiler.
Makefile needs to change with corresponding EOS module
and timer subroutine. (For some PC Windows-based compilers,
see *Remarks below.)

Step 7: Type: 'make' (such as for SUN workstation)

*Remarks: for many PC Windows-based compilers, special compiler options may be
required to generate 64-bit code at compile time. For example, using COMPAQ
Visual Fortran compiler 6.6, the user needs to select proper window
boxs. The following steps must be followed:

(1) Developer Studio

Start DIGITAL/Compaq Visual Fortran's Developer Studio.

(2) Create new Project

Select <File>, <New...>
Select <Projects>, <Win32 Console Application>,
<Project name:> treact
<Location:> C:\Program Files\Microsoft Visual Studio\MyProjects\treact <default, OK>
Check <Create new workspace>, <Platforms:> Win32, <OK>

(3) Copy source files

Copy all source files (as mentioned above in Steps 2, 4 and 5 but in subdirectory ~/integer not/integer*8) to the defaults location, or,
C:\Program Files\Microsoft Visual Studio\MyProjects\treact

(4) Add source files

Select <Project>, <Add to project>, <Files...>
Select all source files (a total of 18 files):

(5) Compiler settings

Select <Project>, <Settings...>
<Settings for>: Win32 Release
<General>, <Not Using MFC>
<Intermediate:> blank
<Output files:> blank

<Fortran>
<Category>: General
<Optimization level:> Optimize for Speed
In the <Project option> window, add the following option:

```
        /real_size:64 (in fact, IMPLICIT DOUBLE PRECISION (A-H, O-Z) statements
        are coded in the source files, without this option the executable code
        is still working, but this option does not result in additional
        computing time)
In the <Project option> window, delete the following option:

        /check:bounds
Leave all other settings unchanged

<Link>
<Output File Name:> treact.exe (or other convenient name for executable)
<OK>

(6) Compile and Link
--------------------
<Build>, <Build treact.exe>
    After this step, file treact.exe will be found in ~\MyProjects\treact\debug

(7) Miscellaneous
-----------------
A new executable must be built for each EOS module.

To redimension TOUGH2, adjust parameter statements in file T2 and chempar23.inc:
<File>, <Open...>
<File name:> T2 or chempar23.inc
Modify parameter statements, save file, and rebuild treact.
```

==========

3. EXECUTION

3.1. Execution

Step 1 Create a directory in user's computer.

Step 2: Prepare a total of four input files (or copy files from sample problems and then modify): flow.inp, solute.inp, chemical.inp, and chemical database input (user specified name).

Step 3 Type: treact, if this executable file is in the current directory.

3.2. Test

Users should run several of the sample problems to check on proper code installation. Due to machine-dependent roundoff, TOUGHREACT may produce slightly different results on different computers. For same-size time steps, all primary variables (pressure P, temperature T, saturation S, etc.) and their changes (DX1, DX2,...) should agree to typically four digits or better (file flow.out). However, on different computers the iteration sequence for a time step may be slightly different because of roundoff, and occasionally a different number of iterations may be required for convergence. If automatic time stepping is used, a different number of iterations for convergence may subsequently cause different-size time steps to be taken; naturally this will then produce somewhat larger discrepancies in results because of different time truncation errors.

Of all the numbers processed by TOUGHREACT, the most sensitive are the residuals, i.e. the differences between left-hand sides (accumulation terms) and right-hand sides of the governing equations.

During the Newton-Raphson iteration process these residuals are reduced to smaller and smaller values, until they drop below specified convergence tolerances. As convergence is approached, the residuals are subject to increasingly severe numerical cancellation, arising from subtracting two numbers with diminishing difference. Maximum residuals are (optionally) printed in file "flow.out" during the iteration process as "MAX. RES.", and are also printed in the header of a full time step printout (as "MAX. RES." or "RERM"). These numbers can serve as a convenient check when evaluating reproducibility of code applications. Small numerical differences due to roundoff etc. will first show up in different values for "MAX. RES.", long before giving any visible changes in primary variables or their increments.

****

TOUGHREACT is documented in:

T. Xu, E. Sonnenthal, N. Spycher, and K. Pruess, TOUGHREACT UserÆs Guide: A Simulation Program for Non-isothermal Multiphase Reactive Geochemical Transport in Variably Saturated Geologic Media, Lawrence Berkeley National Laboratory Report LBNL-55460, July 2004.

TOUGH2 V2 is documented in:

K. Pruess, C. Oldenburg, and G. Moridis, TOUGH2 User's Guide, Version 2.0, Lawrence Berkeley National Laboratory Report LBNL-43134, November 1999.

```
*************************************************************************

Distribution of the TOUGHREACT code is handled by

   Energy Science and Technology Software Center
   P.O. Box 1020
   Oak Ridge, Tennessee 37831
   U.S.A.

   phone (865) 576-2606
   fax   (865) 576-6436
   email: estsc@adonis.osti.gov
   WorldWideWeb: http://www.osti.gov/estsc/

The code development team can be reached as follows

   TIANFU XU
   Mail Stop 90-1116
   Lawrence Berkeley National Lab.
   Berkeley, CA 94720
   U.S.A.

   fax    (510) 486-5686
   email: Tianfu_Xu@lbl.gov

Users are requested to tell us about any bugs that may be encountered.
We also like to hear about code improvements and enhancements; send
e-mail to Tianfu_Xu@lbl.gov.

*************************************************************************
* Additional information is available on the TOUGH2 homepage on the web *
*                                                                       *
*                http://www-esd.lbl.gov/TOUGH2/                         *
```

****

.....
.....READ.ME.....READ.ME.....READ.ME.....READ.ME.....
.....
.....Update 10/04.....
.....

APPENDIX B

OUTPUT FILE COMPARISONS

Validation Test Problem 6.3.1

Flow.out comparison:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P1_validation_test_run\flow.out (242242 bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P1_EOS9_kd-decay\flow.out (239700 bytes)

8c8
<                ---------- Version 1.0 (YMP Q V3.1) -----------
---
>                ------------------ Version 1.0 -------------------
74,80c74,80
<  FILE *VERS* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *MESH* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *INCON* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *GENER* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *SAVE* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *LINEQ* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *TABLE* DOES NOT EXIST --- OPEN AS A NEW FILE
---
>  FILE *VERS*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *MESH*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *INCON* EXISTS --- OPEN AS AN OLD FILE
>  FILE *GENER* EXISTS --- OPEN AS AN OLD FILE
>  FILE *SAVE*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *LINEQ* EXISTS --- OPEN AS AN OLD FILE
>  FILE *TABLE* EXISTS --- OPEN AS AN OLD FILE
2496c2496
<  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =      1.000 SEC-- CALCULATION TIME =
1.000 SEC-- DATA INPUT TIME =    0.000 SEC
---
>  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =      2.000 SEC-- CALCULATION TIME =
2.000 SEC-- DATA INPUT TIME =    0.000 SEC
```

Solute.out comparison:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P1_validation_test_run\solute.out (6564 bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P1_EOS9_kd-decay\solute.out (6427 bytes)

The files are identical
```

Chemical.out comparison results:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P1_validation_test_run\chemical.out (5978 bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P1_EOS9_kd-decay\chemical.out (5866 bytes)

The files are identical
```

***Iter.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P1_validation_test_run\iter.dat (10263 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P1_EOS9_kd-decay\iter.dat (10128 bytes)

The files are identical

kdd_conc.dat comparison:

Compare: (<)D:\TOUGHREACT\sample-problems\P1_validation_test_run\kdd_conc.dat (30651 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P1_EOS9_kd-decay\kdd_conc.dat (30400 bytes)

The files are identical

kdd_gas.dat comparison:

Compare: (<)D:\TOUGHREACT\sample-problems\P1_validation_test_run\kdd_gas.dat (10333 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P1_EOS9_kd-decay\kdd_gas.dat (10084 bytes)

The files are identical

kdd_min.dat domparison:

Compare: (<)D:\TOUGHREACT\sample-problems\P1_validation_test_run\kdd_min.dat (15973 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P1_EOS9_kd-decay\kdd_min.dat (15722 bytes)

The files are identical

kdd_tim.dat comparison:

Compare: (<)D:\TOUGHREACT\sample-problems\P1_validation_test_run\kdd_tim.dat (3953 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P1_EOS9_kd-decay\kdd_tim.dat (3916 bytes)

The files are identical

Validation Test Problem 6.3.2

***Flow.out* comparison**:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P2_validation_test_run\flow.out (261438
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P2_EOS9_Aquia-aquifer\flow.out (258939 bytes)

8c8
<                ---------- Version 1.0 (YMP Q V3.1) ----------
---
>                  ---------- Version 1.0 ----------
74,80c74,80
<  FILE *VERS* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *MESH* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *INCON* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *GENER* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *SAVE* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *LINEQ* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *TABLE* DOES NOT EXIST --- OPEN AS A NEW FILE
---
>  FILE *VERS*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *MESH*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *INCON* EXISTS --- OPEN AS AN OLD FILE
>  FILE *GENER* EXISTS --- OPEN AS AN OLD FILE
>  FILE *SAVE*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *LINEQ* EXISTS --- OPEN AS AN OLD FILE
>  FILE *TABLE* EXISTS --- OPEN AS AN OLD FILE
2453c2453
<  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =    12.000 SEC--
CALCULATION TIME =     12.000 SEC-- DATA INPUT TIME =    0.000 SEC
---
>  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =    22.000 SEC--
CALCULATION TIME =     22.000 SEC-- DATA INPUT TIME =    0.000 SEC
```

***Solute.out* comparison**:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P2_validation_test_run\solute.out (4235
bytes)
with: (>)D:\TOUGHREACT\sample-problems\P2_EOS9_Aquia-aquifer\solute.out (4140 bytes)

The files are identical
```

***Chemical.out* comparison**:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P2_validation_test_run\chemical.out (9431
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P2_EOS9_Aquia-aquifer\chemical.out (9261
bytes)

The files are identical
```

***ITER.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P2_validation_test_run\iter.dat (14232 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P2_EOS9_Aquia-aquifer\iter.dat (14048 bytes)

The files are identical

***aqui_con.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P2_validation_test_run\aqui_con.dat (16071 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P2_EOS9_Aquia-aquifer\aqui_con.dat (15962 bytes)

The files are identical

***aqui_gas.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P2_validation_test_run\aqui_gas.dat (4357 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P2_EOS9_Aquia-aquifer\aqui_gas.dat (4250 bytes)

The files are identical

***aqui_min.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P2_validation_test_run\aqui_min.dat (13775 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P2_EOS9_Aquia-aquifer\aqui_min.dat (13664 bytes)

The files are identical

***aqui_tim.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P2_validation_test_run\aqui_tim.dat (71751 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P2_EOS9_Aquia-aquifer\aqui_tim.dat (71443 bytes)

The files are identical

***Flow.out* comparison:**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P3_validation_test_run\flow.out (79594
bytes)
with: (>)D:\TOUGHREACT\sample-problems\P3_EOS3_YM-calcite\flow.out (78548 bytes)

8c8
<                ---------- Version 1.0 (YMP Q V3.1) -----------
---
>                ------------------ Version 1.0 -------------------
74,80c74,80
<  FILE *VERS* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *MESH* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *INCON* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *GENER* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *SAVE* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *LINEQ* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *TABLE* DOES NOT EXIST --- OPEN AS A NEW FILE
---
>  FILE *VERS*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *MESH*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *INCON* EXISTS --- OPEN AS AN OLD FILE
>  FILE *GENER* EXISTS --- OPEN AS AN OLD FILE
>  FILE *SAVE*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *LINEQ* EXISTS --- OPEN AS AN OLD FILE
>  FILE *TABLE* EXISTS --- OPEN AS AN OLD FILE
406c406
<  END OF TOUGH2 INPUT JOB --- ELAPSED TIME =   1.0000 SECONDS
---
>  END OF TOUGH2 INPUT JOB --- ELAPSED TIME =   0.0000 SECONDS
1000c1000
<  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =      4.000 SEC-- CALCULATION
TIME =      3.000 SEC-- DATA INPUT TIME =     1.000 SEC
---
>  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =      7.000 SEC-- CALCULATION
TIME =      7.000 SEC-- DATA INPUT TIME =     0.000 SEC
```

***solute.out* comparison:**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P3_validation_test_run\solute.out (6755
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P3_EOS3_YM-calcite\solute.out (6614 bytes)

The files are identical
```

***chemical.out* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P3_validation_test_run\chemical.out (39729 bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P3_EOS3_YM-calcite\chemical.out (38868 bytes)

The files are identical

***iter.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P3_validation_test_run\iter.dat (3216 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P3_EOS3_YM-calcite\iter.dat (3168 bytes)

```
25,37c25,37
<        8  0.808046E-05    1    1    18   11.983     0    0.000  0.14815E-02
<        9  0.161926E-04    1    1    18   12.283     0    0.000  0.29630E-02
<       10  0.324169E-04    1    1    19   12.083     0    0.000  0.59259E-02
<       11  0.648655E-04    1    1    19   11.800     0    0.000  0.11852E-01
<       12  0.129763E-03    1    1    19   11.100     0    0.000  0.23704E-01
<       13  0.259557E-03    2    1    18   10.033     0    0.000  0.47407E-01
<       14  0.519146E-03    1    1    19    9.067     0    0.000  0.94815E-01
<       15  0.103832E-02    1    1    19    8.567     0    0.000  0.18963E+00
<       16  0.207668E-02    1    1    20    8.283     0    0.000  0.37926E+00
<       17  0.415339E-02    1    1    20    8.300     0    0.000  0.75852E+00
<       18  0.830681E-02    3    1    20    8.067     0    0.000  0.15170E+01
<       19  0.166137E-01    2    1    20    8.867     0    0.000  0.30341E+01
<       20  0.332273E-01    2    1    19    8.683     0    0.000  0.60681E+01
---
>        8  0.808046E-05    3    1    18   12.000     0    0.000  0.14815E-02
>        9  0.161926E-04    1    1    18   12.250     0    0.000  0.29630E-02
>       10  0.324169E-04    1    1    19   12.083     0    0.000  0.59259E-02
>       11  0.648655E-04    2    1    19   11.883     0    0.000  0.11852E-01
>       12  0.129763E-03    1    1    19   11.017     0    0.000  0.23704E-01
>       13  0.259557E-03    2    1    18   10.083     0    0.000  0.47407E-01
>       14  0.519146E-03    1    1    19    9.033     0    0.000  0.94815E-01
>       15  0.103832E-02    2    1    19    8.583     0    0.000  0.18963E+00
>       16  0.207668E-02    3    1    20    8.283     0    0.000  0.37926E+00
>       17  0.415339E-02    1    1    20    8.333     0    0.000  0.75852E+00
>       18  0.830681E-02    2    1    20    8.017     0    0.000  0.15170E+01
>       19  0.166137E-01    3    1    20    8.933     0    0.000  0.30341E+01
>       20  0.332273E-01    2    1    19    8.583     0    0.000  0.60681E+01
```

***YMC-conc.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P3_validation_test_run\YMC_conc.dat (20463 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P3_EOS3_YM-calcite\YMC_conc.dat (20330 bytes)

The files are identical

***YMC_gas.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P3_validation_test_run\YMC_gas.dat (8430 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P3_EOS3_YM-calcite\YMC_gas.dat (8297 bytes)

The files are identical

***YMC_min.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P3_validation_test_run\YMC_min.dat (20417 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P3_EOS3_YM-calcite\YMC_min.dat (20283 bytes)

The files are identical

***time.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P3_validation_test_run\time.dat (1037 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P3_EOS3_YM-calcite\time.dat (1024 bytes)

The files are identical

Validation Test Problem 6.3.4

***flow.out* comparison:**

A copy of the *flow.out* file was not provided as part of the program disk. Therefore, no comparison was possible.

***solute.out* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P4_validation_test_run\solute.out (246083 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P4_EOS4_heat-test\solute.out (241512 bytes)

The files are identical

***chemical.out* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P4_validation_test_run\chemical.out (62623 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P4_EOS4_heat-test\chemical.out (61337 bytes)

The files are identical

***iter.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P4_validation_test_run\iter.dat (2973 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P4_EOS4_heat-test\iter.dat (2928 bytes)

The files are identical

***tec_conc.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P4_validation_test_run\tec_conc.out (1993995 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P4_EOS4_heat-test\tec_conc.out (1985006 bytes)

The files are identical

***tec_gas.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P4_validation_test_run\tec_gas.out (592926 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P4_EOS4_heat-test\tec_gas.out (583937 bytes)

The files are identical

***tec_min.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P4_validation_test_run\tec_min.out (3817217 bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P4_EOS4_heat-test\tec_min.out (3808227 bytes)

The files are identical

***time.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P4_validation_test_run\time.dat (47609 bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P4_EOS4_heat-test\time.dat (47520 bytes)

The files are identical

Validation Test Problem 6.3.5

Flow.out **comparison:**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P5_validatoin_test_run\flow.out (253970
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P5_ECO2_1D-radial\flow.out (251462 bytes)

2507c2507
<  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =     75.000 SEC--
CALCULATION TIME =     75.000 SEC-- DATA INPUT TIME =    0.000 SEC
---
>  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =    134.000 SEC--
CALCULATION TIME =    134.000 SEC-- DATA INPUT TIME =    0.000 SEC
```

solute.out **comparison**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P5_validatoin_test_run\solute.out (10491
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P5_ECO2_1D-radial\solute.out (10282 bytes)

The files are identical
```

chemical.out **comparison:**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P5_validatoin_test_run\chemical.out (26593
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P5_ECO2_1D-radial\chemical.out (26176 bytes)

The files are identical
```

iter.dat **comparison**:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P5_validatoin_test_run\iter.dat (6132 bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P5_ECO2_1D-radial\iter.dat (6048 bytes)

The files are identical
```

co2d_conc.dat **comparison:**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P5_validatoin_test_run\co2d_conc.dat
(134514 bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P5_ECO2_1D-radial\co2d_conc.dat (133849
bytes)

The files are identical
```

***co2d_gas.dat* comparison:**

A copy of the co2d_gas.dat file was not provided as part of the program disk. Therefore, no comparison was possible.

***co2d_min.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P5_validatoin_test_run\co2d_min.dat (182116 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P5_ECO2_1D-radial\co2d_min.dat (181451 bytes)

The files are identical

***co2d_tim.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P5_validatoin_test_run\co2d_tim.dat (22115 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P5_ECO2_1D-radial\co2d_tim.dat (22054 bytes)

The files are identical

Validation Test Problem 6.3.6

Flow.out **comparison:**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P6_validation_test_run\flow.out (197727
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P6_EOS9_copper\flow.out (195524 bytes)

8c8
<                ---------- Version 1.0 (YMP Q V3.1) ----------
---
>                ------------------ Version 1.0 -------------------
74,80c74,80
<  FILE *VERS* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *MESH* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *INCON* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *GENER* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *SAVE* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *LINEQ* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *TABLE* DOES NOT EXIST --- OPEN AS A NEW FILE
---
>  FILE *VERS*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *MESH*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *INCON* EXISTS --- OPEN AS AN OLD FILE
>  FILE *GENER* EXISTS --- OPEN AS AN OLD FILE
>  FILE *SAVE*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *LINEQ* EXISTS --- OPEN AS AN OLD FILE
>  FILE *TABLE* EXISTS --- OPEN AS AN OLD FILE
2157c2157
<  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =    50.000 SEC--
CALCULATION TIME =     50.000 SEC-- DATA INPUT TIME =    0.000 SEC
---
>  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =    91.000 SEC--
CALCULATION TIME =     91.000 SEC-- DATA INPUT TIME =    0.000 SEC
```

solute.out **comparison:**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P6_validation_test_run\solute.out (8022
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P6_EOS9_copper\solute.out (7859 bytes)

The files are identical
```

chemical.out **comparison**:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P6_validation_test_run\chemical.out (23868
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P6_EOS9_copper\chemical.out (23470 bytes)

The files are identical
```

***iter.dat* comparison:**

A copy of the iter.dat file was not provided as part of the program disk. Therefore, no comparison was possible.

***Amic_aqu.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P6_validation_test_run\Amic_aqu.dat (43401 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P6_EOS9_copper\Amic_aqu.dat (43160 bytes)

The files are identical

***Amic_gas.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P6_validation_test_run\Amic_gas.dat (12749 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P6_EOS9_copper\Amic_gas.dat (12508 bytes)

The files are identical

***Amic_ite.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P6_validation_test_run\Amic_ite.dat (8400 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P6_EOS9_copper\Amic_ite.dat (8288 bytes)

The files are identical

***Amic_sod.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P6_validation_test_run\Amic_sod.dat (57168 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P6_EOS9_copper\Amic_sod.dat (56926 bytes)

The files are identical

***Amic_tim.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P6_validation_test_run\Amic_tim.dat (1752 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P6_EOS9_copper\Amic_tim.dat (1738 bytes)

The files are identical

Validation Test Problem 6.3.7

***Flow.out* comparison**:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P7_validation_test_run\flow.out (483667
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P7_EOS2_LVC\flow.out (478803 bytes)

8c8
<                ---------- Version 1.0 (YMP Q V3.1) ----------
---
>                ------------------ Version 1.0 -------------------
74,80c74,80
<  FILE *VERS* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *MESH* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *INCON* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *GENER* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *SAVE* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *LINEQ* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *TABLE* DOES NOT EXIST --- OPEN AS A NEW FILE
---
>  FILE *VERS*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *MESH*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *INCON* EXISTS --- OPEN AS AN OLD FILE
>  FILE *GENER* EXISTS --- OPEN AS AN OLD FILE
>  FILE *SAVE*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *LINEQ* EXISTS --- OPEN AS AN OLD FILE
>  FILE *TABLE* EXISTS --- OPEN AS AN OLD FILE
4818c4818
<  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =    41.000 SEC--
CALCULATION TIME =     41.000 SEC-- DATA INPUT TIME =    0.000 SEC
---
>  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =    75.000 SEC--
CALCULATION TIME =     75.000 SEC-- DATA INPUT TIME =    0.000 SEC
```

***solute.out* comparison**:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P7_validation_test_run\solute.out (25085
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P7_EOS2_LVC\solute.out (24605 bytes)

The files are identical
```

***chemical.out* comparison**:

```
Compare: (<)D:\TOUGHREACT\sample-problems\P7_validation_test_run\chemical.out (17062
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P7_EOS2_LVC\chemical.out (16768 bytes)

The files are identical
```

***iter.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P7_validation_test_run\iter.dat (3702 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P7_EOS2_LVC\iter.dat (3648 bytes)

The files are identical

***LVC_conc.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P7_validation_test_run\LVC_conc.dat (180849 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P7_EOS2_LVC\LVC_conc.dat (179636 bytes)

The files are identical

***LVC_gas.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P7_validation_test_run\LVC_gas.dat (79680 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P7_EOS2_LVC\LVC_gas.dat (78467 bytes)

The files are identical

***LVC_min.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P7_validation_test_run\LVC_min.dat (280860 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P7_EOS2_LVC\LVC_min.dat (279646 bytes)

The files are identical

***LVC_tim.dat* comparison**:

Compare: (<)D:\TOUGHREACT\sample-problems\P7_validation_test_run\LVC_tim.dat (7265 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P7_EOS2_LVC\LVC_tim.dat (7234 bytes)

The files are identical

Validation Test Problem 6.3.8

***flow.out* comparison:**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P8_validation_test_run\flow.out (583811
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P8_EOS1_scaling\flow.out (578034 bytes)

8c8
<                ---------- Version 1.0 (YMP Q V3.1) ----------
---
>                ------------------ Version 1.0 -------------------
74,80c74,80
<  FILE *VERS* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *MESH* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *INCON* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *GENER* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *SAVE* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *LINEQ* DOES NOT EXIST --- OPEN AS A NEW FILE
<  FILE *TABLE* DOES NOT EXIST --- OPEN AS A NEW FILE
---
>  FILE *VERS*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *MESH*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *INCON* EXISTS --- OPEN AS AN OLD FILE
>  FILE *GENER* EXISTS --- OPEN AS AN OLD FILE
>  FILE *SAVE*  EXISTS --- OPEN AS AN OLD FILE
>  FILE *LINEQ* EXISTS --- OPEN AS AN OLD FILE
>  FILE *TABLE* EXISTS --- OPEN AS AN OLD FILE
5731c5731
<  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =    22.000 SEC--
CALCULATION TIME =     22.000 SEC-- DATA INPUT TIME =    0.000 SEC
---
>  END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME =    42.000 SEC--
CALCULATION TIME =     42.000 SEC-- DATA INPUT TIME =    0.000 SEC
```

***solute.out* comparison:**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P8_validation_test_run\solute.out (6077
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P8_EOS1_scaling\solute.out (5949 bytes)

The files are identical
```

***chemical.out* comparison:**

```
Compare: (<)D:\TOUGHREACT\sample-problems\P8_validation_test_run\chemical.out (18187
bytes)
  with: (>)D:\TOUGHREACT\sample-problems\P8_EOS1_scaling\chemical.out (17909 bytes)

The files are identical
```

***iter.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P8_validation_test_run\iter.dat (16014 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P8_EOS1_scaling\iter.dat (15808 bytes)

The files are identical

***sca_conc.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P8_validation_test_run\sca_conc.dat (201632 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P8_EOS1_scaling\sca_conc.dat (200525 bytes)

The files are identical

***sca_gas.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P8_validation_test_run\sca_gas.dat (59127 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P8_EOS1_scaling\sca_gas.dat (58022 bytes)

The files are identical

***sca_min.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P8_validation_test_run\sca_min.dat (226523 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P8_EOS1_scaling\sca_min.dat (225415 bytes)

The files are identical

***time.dat* comparison:**

Compare: (<)D:\TOUGHREACT\sample-problems\P8_validation_test_run\time.dat (58314 bytes)
with: (>)D:\TOUGHREACT\sample-problems\P8_EOS1_scaling\time.dat (58132 bytes)

The files are identical