QA: QA

VALIDATION TEST REPORT (VTR)
for
TOUGHREACT Version 2.2

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PRELIMINARY DRAFT
INFORMATION ONLY

CHANGE HISTORY

Revision Number	Effective Date	Description of Change
00	03/12/00	Initial issue of CP1 documents prior to ITSMA review.
01	05/1/00	Initial issue of CP1 documents following ITSMA review. The changes were the correction to the "QA" designator, addition of this Change History, and the resulting change in page numbers.

This Validation Test Report (VTP) 10154-VTP-2.2-01 is based upon Software Activity Plan (SAP) 10154-SAP-2.2-01, and Requirements Document (RD) 10154-RD-2.2-01, the Design Document (DD) 10154-DD-2.2-01, the Installation Test Plan (ITP) 10154-ITP-2.2-01, and the Validation Test Plan (VTP) 10154-VTP-2.2-01. In accordance with AP-SI.1Q, Rev. 2, ICN 4, *Software Management*, the VTR is preceded by the Users Manual (UM) 10154-UM-2.2-01, and represents the final document to be submitted (along with the UM and software media) for Information Technology Software Management Analyst (ITSMA) review for Control Point 2.

1.0 OVERVIEW of REPORT

From the VTP, derived from the RD and DD, there are testable requirements in accordance with the DD, Section II.5. They include regression tests with the previous version to ensure that the new enhancement does not adversely affect the operation of the existing features of the software.

TOUGHREACT V2.2 is an upgrade of TOUGHREACT V2.1 (STN: 10042-2.1-01) (previously baselined and qualified, Spycher et al. 1999). In TOUGHREACT V2.2, the following modifications and additions have been made (see RD) as listed below:

1. All upgrades necessary for consistency with TOUGH2 EOS3 v1.4 (STN: 10007-1.4-01) (Wu et al. 1999): active-fracture model, downstream weighting option, capillary pressure linear extrapolation at low liquid saturations, changes in relative permeability based on a modified Brooks-Corey model;
2. Restart option for reactive transport;
3. New option for calculating gas diffusion coefficients as function of temperature and pressure;
4. Use input tortuosity to weight molecular diffusion coefficients;
5. New options for calculating effective surface areas;
6. New option for precipitation rate law;
7. Time dependent thermal conductivity factors;
8. New conjugate gradient stabilized solver;
9. Carmen-Kozeny porosity-permeability coupling option;
10. Modified output options and formats (separate plot ouput file for gases, option to output gas and mineral amounts in volume fraction, output additional variables such as porosity and permeability in plot files).

According to the VTP, hand-testing was the primary method for software validation for testable requirements 2 to 7, 9 and 10. Regression testing against the previous version TOUGHREACT V2.1 and TOUGH2 EOS3 V1.4 was used for software validation for testable requirements 1 and 8. The test cases (Appendix A, Table 2-1) were taken from the VTP.

2.0 VALIDATION TESTER IDENTIFICATION

N. Spycher performed the tests.

3.0 SPECIAL TOOLS and EQUIPMENT

3.1 Identification of Special Tools and Equipment

No special tools or equipment were necessary to perform these validation tests.

4.0 DOCUMENTATION OF TEST RESULTS FROM EXECUTING THE ITP, VTP

4.1 Information Relevant to the Execution of the ITP

The tests were performed on the platform where development occurred (Appendix A).

4.2 Information Relevant to the Execution of the VTP
The validation followed the VTP and was performed without error (Appendix A).

4.3 Test Results Linked to Unique Test Identifier from VTP
The test results are documented in Appendix A for test problem numbers as shown on Table 1. Appendix B lists file folders where test input/output files are located.

4.4 Pass/Fail Indication Per Unique Test Identifier from VTP
For both the testable requirements and the regression tests, the acceptance criteria were met. Therefore, the code passed all test cases (Appendix A).

5.0 DESCRIPTION OF FAILURE CONDITIONS

5.1 How Failure Conditions Occurred
There were no failures during the installation or the validation tests.

5.2 Failure Resolution
Not applicable (see Section 5.1).

6.0 TEST CONCLUSIONS

6.1 Overall Test Conclusions
Since the code passed all tests (Table 1 and Appendix A), it is considered to have been satisfactorily validated according to the requirements.

6.2 Justification for Allowing Test Exceptions to Stay within This Category
There were no test exceptions.

6.3 Summary of Unit Testing Performed
The software was tested as a whole (i.e. the main code and all routines compiled into one executable code; no units were tested separately).

6.4 General Remarks
The tests were concluded satisfactorily.

7.0 LIMITATIONS AND IMPACTS

7.1 Assumptions, Constraints, Bounds, or Limits
For the geochemical processes considered in this software, the range of the input data determines the limitations.

7.2 Impact of the Results
The results show that the output of the software is within the limitations of the input data, and hence acceptable.

8.0 RELATIONSHIP TO OTHER WORK

This work is not related to any other work other than its predecessor software, TOUGHREACT V2.1. There was no requirement for this code to interface with any other software.

References:

Spycher, N., Sonnenthal, E., Ahlers, R., and Xu, T., *TOUGHREACT V2.1 Software Qualification*, 1999. MOL.20000216.0113

Wu, Y.S., Haukwa, C., and Mukhopadyay S., *TOUGH2 V1.4 and T2R3D V1.4: Verification and Validation Report and User's Manual,* Rev 00, 1999. MOL 20000216.0111

Appendix A - THOUGHREACT V2.2 Verification and Validation Report

1. Introduction

This report presents the results of verification and validation tests to confirm that TOUGHREACT V2.2 has met the QA requirements set forth in the Validation Test Plan. Part of the testing of TOUGHREACT V2.2 relied on running validation/verification tests previously developed for the qualification of V2.1, and ensuring that V2.2 produced equivalent results as V2.1. New test problems have also been developed to verify new features.

TOUGHREACT V2.2 is an upgrade of TOUGHREACT V2.1 (STN: 10042-2.1-01) (previously baselined and qualified, see Spycher et al. 1999).

In V2.2, the following modifications and additions have been made as listed below:

1. All upgrades necessary for consistency with TOUGH2 EOS3 v1.4 (STN: 10007-1.4-01) (Wu et al. 1999): active-fracture model, downstream weighting option, capillary pressure linear extrapolation at low liquid saturations, changes in relative permeability based on a modified Brooks-Corey model;
2. Restart option for reactive transport;
3. New option for calculating gas diffusion coefficients as function of temperature and pressure;
4. Use input tortuosity to weight molecular diffusion coefficients;
5. New options for calculating effective surface areas;
6. New option for precipitation rate law;
7. Time dependent thermal conductivity factors;
8. New conjugate gradient stabilized solver;
9. Carmen-Kozeny porosity-permeability coupling option;
10. Modified output options and formats (separate plot ouput file for gases, option to output gas and mineral amounts in volume fraction, output additional variables such as porosity and permeability in plot files).

2. Requirements And System Limitations

Requirements and limitations of TOUGHREACT V2.2 have not changed since V2.1, and are summarized below.

2.1 Hardware, Operating System, And Compiler Requirements

TOUGHREACT V2.2 has been tested on the following platforms:

Platform	Operating System	Compiler
SUN Ultrasparc systems with single or multiple processors	Solaris SUNOS 5.5.1	SUN f77 (optimization: -O3) Incorrect results are likely if a more aggressive optimization is attempted.
DEC Alpha	DEC-UNIX	DEC F77 with following options: - O4 -warn noalignments -fpe4 -check overflow -assume backslash -check no power -check underflow

Verification of the successful implementation of TOUGHREACT V2.2 on these platforms is demonstrated in Section 4.

2.2 User Requirements

These have not changed from version V2.1. The correct implementation, setup, problem formulation, and interpretation of the results of TOUGHREACT requires knowledge of the basic equations of fluid and heat flow and transport in porous media and a basic understanding of the numerical solution of the partial differential equations that are used to describe these processes. In addition, the formulation of the geochemical problem requires familiarity with geochemical modeling and an in-depth understanding of the system that is being modeled and of the data used for input to the model. The model boundary conditions, time step length, convergence criteria, and grid properties are crucial elements to providing a realistic and accurate solution to a problem. Numerical models can produce erroneous results and therefore must be interpreted with caution.

3. Test Problems and Acceptance Criteria

Table 3-1 lists the requirements and acceptance criteria that were established to validate TOUGHREACT V2.2. "Software validation" ensures that the software meets the requirements specified for it. "Software verification" ensures that algorithms of the program produce the intended output. Verification can be achieved, for example, by simple hand calculations or by comparing program results with analytical solutions. Software verification also fulfills the definition of "software validation" because in order to obtain correct results (e.g., by comparison with an analytical solution), the software must also be able to model the processes of interest in the problem.

The types of requirements and acceptance criteria in Table 2-1 were developed to test the main processes that need to be considered for reactive-transport simulations in unsaturated, non-isothermal, boiling systems. Validation/verification test problems were previously developed for the qualification of TOUGHREACT V2.1. (Spycher et al. 1999). Part of the qualification of TOUGHREACT V2.2 involved running these tests again and ensuring the results were consistent with those of V2.2. New tests have been developed to verify new options and features in V2.2. Results of all tests are presented in Section 4.

Table 3-1. Summary of Validation Problems and Acceptance Criteria for TOUGHREACT V2.2

#	Requirements	Problem Type	Acceptance Criteria	Dimension	Reference
1	Verification of equivalence to TOUGH2 EOS3. Run with V2.2 previous test problems used to qualify V2.1. Ensure both versions yield results within the acceptance criteria.	(a) Flow to a geothermal well (b) Transient heat pipe (c) Two-phase flow	Match results of V2.1 (within 0.1%)	3-D, cylindrical 3-D, cylindrical 1-D, linear	Test Problem 1 in Spycher et al. (1999)
2	Verification of proper chemical mass-balance and mass-action for the chemical solver (no transport) for a fully liquid-saturated case and an unsaturated case. Run with V2.2 previous test problems used to qualify V2.1. Ensure both versions yield results within the acceptance criteria.	(a) Heat water (single phase) from 25 to approximately 100°C at near atmospheric pressure. (b) Heat water and gas (two-phase) from 25 to approximately 100°C at near atmospheric pressure.	(a) Match results of V2.1 (within 0.1%). (b) Match results of V2.1 within 0.1%.	1 grid block (no transport)	Test Problem 2 in Spycher et al. (1999)
3	Verification of evaporative concentration due to boiling. Run with V2.2 a previous test problem used to qualify V2.1. Ensure both versions yield results within the acceptance criteria.	Boil water near 100°C at pressure approximately amospheric.	Match results of V2.1 (within 0.1%).	2 grid blocks (steam transport only)	Test Problem 3 in Spycher et al. (1999)
4	Verification of aqueous transport (advection/diffusion). Run with V2.2 previous test problems used to qualify V2.1. Ensure both versions yield results within the acceptance criteria.	Simulate transport of a chemical tracer at 25°C, 1 bar (version 1.0 test problem 4).	Match results of V2.1 (within 0.1%).	1-D, linear	Test Problem 4 in Spycher et al. (1999)
5	Verification of consistency with new options in TOUGH2 EOS3 V1.4. Run with V2.2 a simulation that uses new features available in EOS3 V1.4. Ensure both versions yield results within the acceptance criteria.	Simulate coupled thermal and hydrological processes induced by a heat source in the unsaturated zone assuming a dual permeability active-fracture model with downstream weighting at one location, capillary pressure linear extrapolation at low liquid saturations, relative permeability based on modified Brooks-Corey model, and new solver.	Match results of V2.1 within 1%.	2-D vertical cross section	This report

6	Verifi[illegible]on of new options for computing mineral effective surface areas and reaction rates. Hand-check that mineral effective surface areas and reaction rates are correctly computed (Equations A-3 through A-8 in the Requirements Document).	Simulate chemical reaction without flo at a constant temperature for a simple problem including 2 minerals, 2 grid blocks (1 fracture and 1 matrix) and five constant time steps. Different rate laws and input surface area units are specified for each mineral, and the active-fracture model is enabled for the fracture grid block. Therefore, all new options are tested in one problem.	Match (at each time t), within 1%, mineral amounts computed with V2.2, with values hand-calculated from computed saturation indexes (at time t) and mineral amounts produced (at time t - dt).	2 grid block (no transport)	This [illegible]ort
7	Verification of porosity-permeability-capillary pressure coupling. Hand-check that porosity, permeability, and capillary pressure changes are correctly computed for matrix and fracture grid blocks (Equations A-9 to A-12 in the Requirements Document).	Simulate heating of a carbonate-bearing solution and precipitation of a hypothetical calcite mineral with a set, arbitrary but intentionally high, molar volume to exaggerate the change in porosity. Run twice: once with starting porosity less than 0.8 (flag for matrix) and once with starting porosity greater than 0.8 (flag for fractures).	Match, within 0.1%, porosity, permeability, and capillary pressure values calculated by V2.2 with values hand-calculated from computed amounts of solid phase produced.	2 grid blocks (no transport)	Similar to Test Problem 7 in Spycher et al. 1999)
8	Verification of gas diffusion coefficient (Equations A-1 and A-2 in the Requirements Document) and gas transport (advection/diffusion) computations using an analytical solution.	Simulate CO_2 transport in a constant, steady state flow field, with option set to calculate the CO_2 diffusion coefficient.	Match concentration ratios ($C/C_{initial}$)computed by V2.2 (as a function of time) with values provided by an analytical solution and hand-calculating the diffusion coefficient, within 5% at ($C/C_{initial}$) values > 0.1.	1-D, linear	Test Problem 8 in Spycher et al. (1999) with new option to calculate the diffusion coefficient.
9	Verification of restart option for reactive transport simulations.	Simulate a complex thermal-hydrological-chemical problem for a given time frame (50 years in this case), then restart the simulation (at 50 years) with a very small initial time step (1 second).	Ensure that the results of the restart simulation (at 50 years + 1 second) match within 1% the results of the original simulation (at the original end time of 50 years).	2-D vertical cross-section	This report.
10	Verification of time-dependent thermal conductivity option.	Simulate a simple linear heat flow problem with 20 constant time steps and option set to vary the thermal conductivity with time.	Hand-calculate thermal conductivities (at each time step) from input factors and conductivities and ensure these values match within 0.1% the values calculated by V2.2.	1-D, linear (4 grid blocks)	This report
11	Verification of output gas and mineral amounts new concentration units	Run Test Problem 1b, but with option enabled to output gas and mineral amounts in volume fraction instead of bars and mol/l_{medium}, respectively.	Back-calculate by hand mineral and gas amounts in mol/l_{medium} and bars, respectively, and compare with results of Test Problem 1. Agreement should be within 0.1%.	1 grid block (no transport)	Test Problem 2 in Spycher et al. (1999)

software validation test problem number

4. Test Problems Results

4.1 TOUGHREACT V2.2 Verification Against TOUGHREACT V2.1 (Test Problems 1 to 4)

Test problems 1 though 4 in Table 2-1 were run with version V2.2, produced results consistent with those of V2.1 and met the acceptance criteria listed in that table (See Scientific Notebook YMP-LBNL-YWT-NS-1.1, p.128-129 and 143-145) (Appendix C).

4.2 TOUGHREACT V2.2 Verification Against TOUGH2 EOS3 V1.4 (Test Problem 5)

Test problem 5 in Table 2-1 was run with version V2.2, produced results consistent with those of TOUGH2 EOS3 V1.4 and met the acceptance criteria listed in that table (See Scientific Notebook YMP-LBNL-YWT-NS-1.1, p.120-123) (Appendix C).

4.3 Verification of Rate Laws and Effective Surface Areas (Test Problem 6)

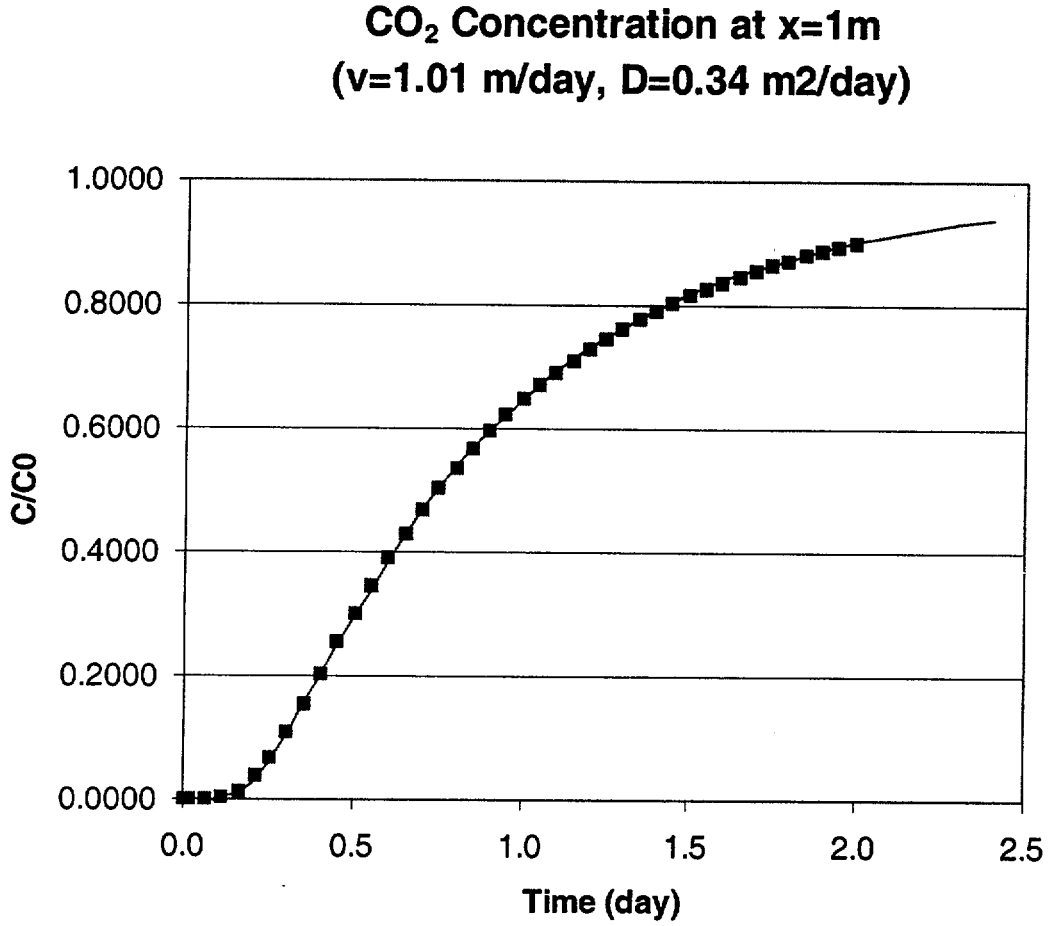
Test problem 6 in Table 2-1 was run with version V2.2 and met the acceptance criteria listed in that table (See Scientific Notebook YMP-LBNL-YWT-NS-1.1, p.137-142) (Appendix C).

4.4 Verification of Porosity-Permeability-Capillary Pressure Coupling (Test Problem 7)

Test problem 7 in Table 2-1 was run with version V2.2 and met the acceptance criteria listed in that table (See Scientific Notebook YMP-LBNL-YWT-NS-1.1, p.130-131) (Appendix C).

4.5 Verification of Gas Diffusion Coefficient and Gas Transport (Test Problem 8)

Test problem 8 in Table 2-1 was run with version V2.2. This problem also verifies the calculation of effective gas diffusion coefficients. There is good agreement between TOUGHREACT V2.2 and the analytical solution (Figure below). Differences between the analytical solution and the results of TOUGHREACT (C/C0) are less than 5% between C/C0 values of 0.1-0.25, then less than 1% at C/C0 values > 0.25, therefore meeting the acceptance criteria listed in Table 2-1 (See Scientific Notebook YMP-LBNL-YWT-NS-1.1, p.134-135) (Appendix C).



Symbols: TOUGHREACT V2.2
Solid line: Analytical Solution (Ogata and Banks, 1961)

4.6 Verification of Restart Option for Reactive Transport Simulations (Test Problem 9)

Test problem 9 in Table 2-1 was run with version V2.2 and met the acceptance criteria listed in that table (See Scientific Notebook YMP-LBNL-YWT-NS-1.1, p.124-127) (Appendix C).

4.7 Verification of Time-Dependent Thermal Conductivity Option (Test Problem 10)

Test problem 10 in Table 2-1 was run with version V2.2 and met the acceptance criteria listed in that table (See Scientific Notebook YMP-LBNL-YWT-NS-1.1, p.132-133) (Appendix C).

4.8 Verification of Gas and Mineral Volume Fraction Printout Option (Test Problem 11)

Test problem 11 in Table 2-1 was run with version V2.2 and met the acceptance criteria listed in that table (See Scientific Notebook YMP-LBNL-YWT-NS-1.1, p.136) (Appendix C).

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5. References

Ogata A. and Banks R.B. 1961. "A solution to the differential equation of longitudinal dispersion in porous media". U.S. Geological Survey Professional Paper 411-A.Spycher, N., Sonnenthal, E.,

Ahlers, R., and Xu, T., *TOUGHREACT V2.1 Software Qualification*, 1999. MOL.20000216.0113

Wu, Y.S., Haukwa, C., and Mukhopadyay S., *TOUGH2 V1.4 and T2R3D V1.4: Verification and Validation Report and User's Manual,* Rev 00, 1999. MOL 20000216.0111

Appendix B - I/O Files For Test Problems and Sample Problems

File Folder Name	Validation Test Problem(*)
geothermal2.2	1a
heat_pipe2.2	1b
2phase_flow2.2	1c
heat_sat1_2.2	2a
heat_unsat1_2.2 heat_unsat2_2.2	2b
boil100_2.2	3
aqtrans2.2	4
qa_vs_eos3_v1.4	5
reac_rates2.2	6
perm-pcap2.2	7
gas_diffus2.2	8
qa_restart2.2	9
k_thermal2.2	10
gas_min_conver2.2	11

Appendix C - Cited Scientific Notebook Pages

Note: All relevant scientific notebook (SN) pages are included in this package. In some instances, the included SN pages cross-reference other pages that are not included here because these were not essential to the documentation of this software.

PROJECT NAME _____ NOTEBOOK NO.

SUPERCEDED by test on p. 143 N.S. 3/10/00

2/11/00 Test Problem #5 in Valid. Test R...

TOUGHREACT V2.2 QA — test against eos3 V1.4

Note added 3/9/00 see addition to this entry on p. 143

Objective Test this version for thermo-hydrological processes only, which include the same new features as those added to eos3 V1.4 (active fracture concept, downstream weighting and saturation-cap. pressure curve truncation at small saturations) N.S. 2/11/00

Method Test against ~~eos3 V1.4~~ eos3 V1.4 (from TOUGH2 V1.4 STN 10007-1.4-0) N.S. 2/14/00 run the same problem using eos3 V1.4 and TOUGHREACT V2.2 (without reactive transport) and compare results.

Acceptance criteria: The results of toughreact V2.2 should match those of eos3 V1.4 within 1 percent (may not be exactly the same because of difference in solvers?)

N.S. 2/11/00 and also new solver (MOP(21)=5; ISOLVC=5)

Problem setup

Use the drift-scale model used for AMR U0110 (YMP-LBNL-DSM-NS-1 p. 33 items 4, 5, and 6) This setup incorporates: active fracture model, sat-pcap curve truncation (ICP = 10 option) and downstream weighting at the PTn-TSw geologic contact, ~~and new solver~~ N.S. 2/11/00 (ISOLVC = 5). Run this 2-D simulation for 100,000 years (essentially steady state) with both toughreact V2.2 and tough2 eos3 V1.4, and compare ~~the SAVE files~~ N.S. 2/14/00 output by both codes. ~~Results are shown below.~~ The state variables (Pressure - P, gas saturation - Sg, and temperature T) output in the SAVE files by both programs.

Results (shown p. 122 & 123)

Both codes yield identical results well within the acceptance criteria of 1% (mostly exact matches).

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PROJECT NAME _____ NOTEBOOK NO. _____

cont'd 2/16/00

Location of test files (exerpts, printouts on p. 122 & 123)

output

on calx /nspycher / treactq2.2_qa/
qa_vs_eos3_v1.4/
eos3_v1.4/ *.* eos3 input/output files
treactq2.2/ *.* toughreact input/output files

Note: these tests were run on calx with a toughreact 2.2 and eos3 1.4 versions compiled on calx (Dec Alpha)

Location of source codes (frozen since 11/ N.S. 2/16/00

eos3 v1.4 (Q version, used executable t2eos3l.exe compiled for Dec Alpha provided by Y.S. Wu at LBNL)

toughreact v2.2 (frozen since 11/12/1999) on hydra:
/usersraid/esonn/t2src/toughreact_2.2q/

*.f (fortran source files - see list of routines used in file "make file")

treactq2.2 (executable, for hydra (Sun Sparc) - note that for the tests described here, the source files were recompiled on calx - see N.S. 2/16/00 ~~calx:/usr/esonn/t2src~~ calx/usr/esonn/t2src/toughreactq-2.2c

over →

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SAVE file output from eos3 V1.4

INCON -- INITIAL CONDITIONS FOR 2216 ELEMENTS AT TIME 0.315570E+13

P 10+Sg T

F 1
0.8856506995806E+05 0.1097243355907E+02 0.2457192330461E+02 0.2756644092804E-01 0.2756644092804E-01
M 1
0.8856506988024E+05 0.1004475101517E+02 0.2457192330655E+02 0.9552489848261E+00 0.9552489848261E+00
F 2
0.8856639258206E+05 0.1097243444916E+02 0.2457376822205E+02 0.2756555083738E-01 0.2756555083738E-01
M 2
0.8856639251093E+05 0.1004481733163E+02 0.2457376822378E+02 0.9551826683682E+00 0.9551826683682E+00
F 3
0.8856781429549E+05 0.1097243500918E+02 0.2457575115650E+02 0.2756499081808E-01 0.2756499081808E-01
M 3
0.8856781422300E+05 0.1004488976200E+02 0.2457575115821E+02 0.9551102380042E+00 0.9551102380042E+00
...
F 535
0.8815286191343E+05 0.1097632784463E+02 0.2383946588168E+02 0.2367215537109E-01 0.2367215537109E-01
M 535
0.8815286172707E+05 0.1019210351040E+02 0.2383946595997E+02 0.8078964895993E+00 0.8078964895993E+00
F 536
0.8815286198662E+05 0.1097632762587E+02 0.2383946595393E+02 0.2367237412686E-01 0.2367237412686E-01
M 536
0.8815286180025E+05 0.1019210564361E+02 0.2383946603223E+02 0.8078943563886E+00 0.8078943563886E+00
...
F1106
0.9126522847761E+05 0.1090066356412E+02 0.2984890144874E+02 0.9933643588119E-01 0.9933643588119E-01
M1106
0.9126654509283E+05 0.1003482947261E+02 0.2984890763196E+02 0.9651705273913E+00 0.9651705273913E+00
F1107
0.9168634263024E+05 0.1090036093176E+02 0.3100673220947E+02 0.9963906824318E-01 0.9963906824318E-01
M1107
0.9170202814498E+05 0.1002485459060E+02 0.3100673922328E+02 0.9751454093956E+00 0.9751454093956E+00
tp001
0.8633854113471E+05 0.1099000000000E+02 0.1768000000000E+02 0.1000000000000E 01 0.1000000000000E-01
bt001
0.9200000000000E+05 0.1000001000000E+02 0.3168000000000E+02 0.9999900000000E+00 0.9999900000000E+00
+++
90 457 46 0.00000000E+00 0.31557000E+13

122 PROJECT NAME NOTEBOOK NO.

SIGNATURE
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DATE 2/16/2000
DATE 19

PROJECT NAME

NOTEBOOK NO.

SAVE file output from tough react V2.2

```
INCON -- INITIAL CONDITIONS FOR 2216 ELEMENTS AT TIME  0.315570E+13
F   1             0.99000000E+00 0.27570000E-12 0.27570000E-12 0.27570000E-12
 0.8856506995806E+05 0.1097243355907E+02 0.2457192330461E+02
M   1             0.11000000E+00 0.40700000E-17 0.40700000E-17 0.40700000E-17
 0.8856506988024E+05 0.1004475101517E+02 0.2457192330655E+02
F   2             0.99000000E+00 0.27570000E-12 0.27570000E-12 0.27570000E-12
 0.8856639258206E+05 0.1097243444916E+02 0.2457376822205E+02
M   2             0.11000000E+00 0.40700000E-17 0.40700000E-17 0.40700000E-17
 0.8856639251093E+05 0.1004481733163E+02 0.2457376822378E+02
F   3             0.99000000E+00 0.27570000E-12 0.27570000E-12 0.27570000E-12
 0.8856781429549E+05 0.1097243500918E+02 0.2457575115650E+02
M   3             0.11000000E+00 0.40700000E-17 0.40700000E-17 0.40700000E-17
 0.8856781422300E+05 0.1004488976200E+02 0.2457575115821E+02

F 535             0.99000000E+00 0.54950000E-12 0.54950000E-12 0.54950000E-12
 0.8815286191343E+05 0.1097632784463E+02 0.2383946588168E+02
M 535             0.15400000E+00 0.30830000E-16 0.30830000E-16 0.30830000E-16
 0.8815286172707E+05 0.1019210351040E+02 0.2383946595997E+02
F 536             0.99000000E+00 0.54950000E-12 0.54950000E-12 0.54950000E-12
 0.8815286198662E+05 0.1097632762587E+02 0.2383946595393E+02
M 536             0.15400000E+00 0.30830000E-16 0.30830000E-16 0.30830000E-16
 0.8815286180025E+05 0.1019210564361E+02 0.2383946603223E+02

F1106             0.99000000E+00 0.31230000E-13 0.31230000E-13 0.31230000E-13
 0.9126522847761E+05 0.1090066356412E+02 0.2984890144874E+02
M1106             0.33100000E+00 0.60690000E-17 0.60690000E-17 0.60690000E-17
 0.9126654509283E+05 0.1003482947261E+02 0.2984890763196E+02
F1107             0.99000000E+00 0.31230000E-13 0.31230000E-13 0.31230000E-13
 0.9168634263024E+05 0.1090036093176E+02 0.3100673220947E+02
M1107             0.33100000E+00 0.60690000E-17 0.60690000E-17 0.60690000E-17
 0.9170202814498E+05 0.1002485459060E+02 0.3100673922328E+02
tp001             0.20000000E+00 0.10000000E-12 0.10000000E-12 0.10000000E-12
 0.8633854113471E+05 0.1099000000000E+02 0.1768000000000E+02
bt001             0.28000000E+00 0.47000000E-15 0.47000000E-15 0.47000000E-15
 0.9200000000000E+05 0.1000001000000E+02 0.3168000000000E+02
+++
    97  453   46 0.00000000E+00 0.31557000E+13
```

Pressure (P), gas saturations (Sg) and temperatures (T) match well within the acceptance criteria of 1% (mostly exact matches).

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PROJECT NAME ~~Test Problem # 9 in Val. Test Rep.~~ N.S. 3/10/00 NOTEBOOK NO.

2/16/00 TOUGHREACT V 2.2 QA – test ~~age~~ N.S. 2/16/00 restart option

Objective: test the option that allows restarting a simulation (with chemical reaction) ~~after~~ N.S. 2/16/00 from some point where the simulation was ended. This option was initially implemented by T. Xu then debugged/modified by myself & E. Sonnenthal. It make use of the SAVECHEM file, which play the same role as the SAVE file (see tough2 user's guide) but for chemical data instead of thermo-hydrological data

Method: run a simulation (with reactive transport) up to a certain end time (t_{end}). Restart at that point with a very small time step (Δt) ~~(so that $t_o \cong t_o + \Delta t$ with t_o = restarting time~~ N.S. 2/16/00 such that $t_{end} = t_{restart} \cong t_{restart} + \Delta t$ and compare the output chemistry data in the TEC_MIN.DAT, TEC_CONC.DAT, and TEC_GAS.DAT files at t_{end} and ~~$t_{restart} + \Delta t$~~. Note, there is no way to compare the chemistry data exactly at $t_{restart}$ because after a restart, full chemical speciation calculations only occur after the first time step.

Note added 3/10/00 N.S.: for the final re-run of this test (see p. 47) the mol. weights in the database had to be multiplied by 1000 to yield the correct results. This run thc6-16-25-4 since the ... comparable ... mol. weight unit ... [illegible]

Notes on this restart option (for info only)

TOUGHREACT V 2.2 outputs a SAVECHEM file at the same time a SAVE file (see tough2 user's guide) is created. A restart run is conducted by copying SAVE to INCON, and SAVECHEM to INCHEM, then copying the end time value at the bottom of the INCON file (last value) over the starting time value (one before last value at the bottom of the INCON file)

Problem setup

Use the 2-D drift-scale model used for AMR U0110 (YMP-LBNL-DSM-NS-1 p. 36 and 37, items 1, 2 ~~and~~ N.S. 2/16/00 – pick one of the 0–50 years runs). Restart this run with a Δt = 1 second ~~and an end time = $t_{restart} + \Delta t$.~~ N.S. 2/16/00 Set run

pick up thc6-16-25-4 (YMP-LBNL-DSM-NS-1, p. 42) N.S. 2/16/00

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Set run flags appropriately so that the ~~TEC~~ TEC_GAS.DAT TEC_MIN.DAT and TEC_CONC.DAT files get printed out. To be able to specify $\Delta t = 1$ second, reset starting time = 0 in the FLOW.INP and INCHEM file and leave INCON as-is (with tstart = 0). ~~This is~~ N.S. 2/16/00 because the restart at 50 years would N.S. 2/16/00 otherwise require ~~t restart = 50 years ≈ 1.5768 N.S. E+9 2/16/00 seconds~~ and specify end time = 1 second. We cannot ~~do this if we~~ N.S. 2/16/00 set the starting time at its original value of 50 years (input as 1.5768 E+9 seconds) because there are not enough input digits spaces in the input file N.S. 4/4/00 to specify an end time of 1.5768 E+9 + 1 second.

Acceptance criteria Model output data (thermal, hydrological, and chemical data in the TEC_CONC.DAT, TEC_MIN.DAT and TEC_GAS.DAT ~~files~~ N.S. 2/16/00 file) at the last time step of the original run should match within 1% those same data for the restart run (note: this criteria does not apply to mineral abundance which are so small that they approach the machine precision limit, typically less than 10^{-12}). Note: the data cannot match exactly because we are comparing results at t and at t + 1 second.

Results

Essentially perfect match well within the acceptance criteria, as ~~shown~~ next pages N.S. 2/16/00 below for a few arbitrarily selected points.

Location of test files

On calx (tests were run on calx)
original run (not reran here):
calx/usr/mspycher/seep_99/thc_runs/thc_16.25_4/*.*

Restart test run:
calx/usr/mspycher/treactq2.2_qa/qa_restart2.2/1/*.*

Code location: see p. 121

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compare.dat

Excerpts from TEC_CONC.DAT, TEC_MIN.DAT and TEC_GAS.DAT file for
arbitrarily selected points in these files.
Comparison between original results at t=50 years and restart results (at t=50 years + 1 second)
Original data is from run thc6_16_25_4 (at 50 years)

VARIABLES =X,Y,Z,SL,T,pH,logfo2,ca+2 ,mg+2 ,na+ ,cl- ,sio2(aq) ,hco3- ,so4-2
,k+ ,alo2- ,f- ,hfeo2 ,

ORIGINAL RESULTS:

2.143 0.000 -1.879 0.0266 75.229 8.8833 0.000 0.5846E-04 0.2568E-05 0.2575E-01
0.1052E-01 0.7007E-02 0.3997E-02 0.3848E-02 0.1925E-03 0.4302E-10 0.1441E-03 0.1744E-09
2.143 0.000 -1.879 0.9862 75.230 8.8238 0.000 0.2787E-04 0.3274E-06 0.9923E-02
0.4001E-02 0.1969E-02 0.2020E-02 0.1462E-02 0.8197E-04 0.1069E-06 0.5486E-04 0.1416E-09

10.890 0.000 -13.080 0.0404 51.146 8.4370 0.000 0.1604E-03 0.7164E-07 0.7094E-02
0.3257E-02 0.3538E-02 0.1280E-02 0.1192E-02 0.3252E-04 0.1996E-11 0.4468E-04 0.1280E-10

1.681 0.000 -2.048 0.0000 76.084 8.3201 0.000 0.2521E-02 0.6996E-03 0.2668E-02
0.3302E-02 0.1175E-02 0.3274E-02 0.1208E-02 0.2047E-03 0.3677E-10 0.4529E-04 0.1156E-11

compare

RESTART RESULTS:

2.143 0.000 -1.879 0.0266 75.229 8.8833 0.000 0.5846E-04 0.2568E-05 0.2575E-01
0.1052E-01 0.7007E-02 0.3997E-02 0.3848E-02 0.1925E-03 0.4302E-10 0.1441E-03 0.1744E-09
2.143 0.000 -1.879 0.9862 75.230 8.8238 0.000 0.2787E-04 0.3274E-06 0.9923E-02
0.4001E-02 0.1969E-02 0.2020E-02 0.1462E-02 0.8197E-04 0.1069E-06 0.5486E-04 0.1416E-09

10.890 0.000 -13.080 0.0404 51.146 8.4370 0.000 0.1604E-03 0.7164E-07 0.7094E-02
0.3257E-02 0.3538E-02 0.1280E-02 0.1192E-02 0.3252E-04 0.1996E-11 0.4468E-04 0.1280E-10

1.681 0.000 -2.048 0.0000 76.045 8.3200 0.000 0.2521E-02 0.6996E-03 0.2668E-02
0.3302E-02 0.1175E-02 0.3274E-02 0.1208E-02 0.2047E-03 0.3677E-10 0.4529E-04 0.1156E-11

VARIABLES =X,Y,Z,T,P,co2(g) ,

ORIGINAL RESULTS:

2.143 0.000 -1.879 75.229 0.8853E+05 0.6486E-03
2.143 0.000 -1.879 75.230 0.8879E+05 0.4089E-03

10.890 0.000 -13.080 51.146 0.8862E+05 0.4483E-03

1.681 0.000 -2.048 76.084 0.1041E+06 0.1056E-04

compare

RESTART RESULTS:

2.143 0.000 -1.879 75.229 0.8853E+05 0.6484E-03
2.143 0.000 -1.879 75.230 0.8879E+05 0.4090E-03

10.890 0.000 -13.080 51.146 0.8862E+05 0.4483E-03

1.681 0.000 -2.048 76.045 0.1041E+06 0.1058E-04

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```
VARIABLES =X,Y,Z,T,PHI,PERM,gypsum     ,goethite   ,microcline,albite-low,anorthite
,smectite-c,smectite-n,smectite-m,smectite-k,illite     ,calcite    ,tridymite ,cristobali,quartz
,sio2(amor.,glass1     ,hematite   ,steller/10,heuland/10,mordeni/10,clinopt/10,kaolinite ,sepiolite
,fluorite   ,
ORIGINAL RESULTS:
     2.143       0.000     -1.879   75.229    0.98988  0.27560E-12  0.0000E+00  0.0000E+00 -0.7340E-07
    -0.9179E-07 -0.8003E-15 -0.1057E-09 -0.4547E-10 -0.1057E-09 -0.4547E-10 -0.3437E-10  0.1116E-03
     0.0000E+00  0.4179E-10  0.0000E+00  0.1267E-04  0.0000E+00  0.2440E-10  0.3309E-06  0.5466E-21
     0.2869E-21  0.8778E-21  0.0000E+00  0.3263E-20  0.8878E-07
     2.143       0.000     -1.879   75.230    0.10999  0.40688E-17  0.0000E+00  0.0000E+00  0.3280E-04
    -0.6760E-04 -0.4636E-09  0.1188E-03  0.1605E-04 -0.6121E-05 -0.3862E-04 -0.5629E-04  0.6315E-05
     0.0000E+00 -0.4714E-06  0.0000E+00  0.0000E+00  0.0000E+00 -0.4131E-12  0.4875E-05  0.1081E-10
     0.2008E-14  0.3613E-11  0.0000E+00  0.1745E-17  0.0000E+00

    10.890       0.000    -13.080   51.146    0.98999  0.27569E-12  0.0000E+00  0.0000E+00 -0.3449E-07
    -0.3084E-07 -0.2644E-15 -0.4760E-10 -0.2047E-10 -0.4760E-10 -0.2047E-10 -0.1547E-10  0.6217E-05
     0.0000E+00  0.3137E-11  0.0000E+00  0.3873E-15  0.0000E+00  0.7629E-13  0.1060E-06  0.5410E-21
     0.2834E-21  0.8688E-21  0.0000E+00  0.9454E-23  0.0000E+00

     1.681       0.000     -2.048   76.084    1.00000  0.00000E+00  0.0000E+00  0.0000E+00  0.0000E+00
     0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
     0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
     0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00

RESTART RESULTS:
     2.143       0.000     -1.879   75.229    0.98975  0.27549E-12  0.0000E+00  0.0000E+00 -0.7340E-07
    -0.9179E-07 -0.8013E-15 -0.1057E-09 -0.4547E-10 -0.1057E-09 -0.4547E-10 -0.3437E-10  0.1116E-03
     0.0000E+00  0.4179E-10  0.0000E+00  0.1267E-04  0.0000E+00  0.2440E-10  0.3309E-06  0.5466E-21
     0.2869E-21  0.8778E-21  0.0000E+00  0.3263E-20  0.8878E-07
     2.143       0.000     -1.879   75.230    0.10998  0.40677E-17  0.0000E+00  0.0000E+00  0.3280E-04
    -0.6760E-04 -0.4636E-09  0.1188E-03  0.1605E-04 -0.6121E-05 -0.3862E-04 -0.5629E-04  0.6315E-05
     0.0000E+00 -0.4714E-06  0.0000E+00  0.0000E+00  0.0000E+00 -0.4131E-12  0.4875E-05  0.1081E-10
     0.2008E-14  0.3613E-11  0.0000E+00  0.1745E-17  0.0000E+00

    10.890       0.000    -13.080   51.146    0.98999  0.27569E-12  0.0000E+00  0.0000E+00 -0.3449E-07
    -0.3084E-07 -0.2651E-15 -0.4760E-10 -0.2047E-10 -0.4760E-10 -0.2047E-10 -0.1547E-10  0.6217E-05
     0.0000E+00  0.3137E-11  0.0000E+00  0.3873E-15  0.0000E+00  0.7629E-13  0.1060E-06  0.5410E-21
     0.2834E-21  0.8688E-21  0.0000E+00  0.9454E-23  0.0000E+00

     1.681       0.000     -2.048   76.045    1.00000  0.00000E+00  0.0000E+00  0.0000E+00  0.0000E+00
     0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
     0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
     0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
```

compare

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2/17/00 TOUGHREACT V2.2. QA ~~Thermal hydrological only~~ regression testing N.S. 2/17/00

Objective: QA ~~The~~ N.S. 2/17/00 ~~TH~~ part of the code by regression testing against Q version 2.1 (STN - 10042 - 2.1 - 00)

Method: run TOUGHREACT V2.2 on same TH problems as run previously with V2.1 for QA purposes and compare results using the unix "diff" command or by superposition of windows using my text editor.

Acceptance criteria: results between V2.2 and V2.1 should be identical (or within output format resolution - say, within 0.1% (arbitrary)).

Test runs and results

(1) Run same tests as described on p. 72, item (10). These are part of test problem #1 in the QA manual for version 2.1 N.S. 2/17/00 Flow to geothermal well: results ~~between~~ of V2.2 and V2.1 are identical

N.S. 3/10/00 Test Problems: 1a in YMP

Heatpipe results of V2.2 and V2.1 are identical. The run finishes properly but there is still an underflow error message popping on the screen as already noted with V1.0 and V2.1.

1b in YMP

1c in YMP

Two-Phase-flow (problems with, and without outer ring). Results of V2.2 and V2.1 are identical. There is still an underflow error message appearing (as noted previously with V2.2 and V1.0) but the runs finish correctly. N.S. 2/17/00

These tests are same tests as those run for TOUGH2 ~~V1.3~~ V1.11 EOS3 qualification (Wu et al., 1996, LBNL report 39490, UC-800) MOL.19970219.0104.

Test problem #2 in YMP

(2) Run the same aqueous transport test as described on p. 71, item 8 (problem #4 of V2.1 QA manual). Results of V2.2 and V2.1 are identical.

(3) Run the same gas transport test as described on p. 71, item 9. For consistency between V2.1 and V2.2, I needed to divide the CO_2 diffusion coefficient used previously with

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V2.1 by the tortuosity read in the FLOW.INP file. This is because V2.2 multiplies the ~~diffusion~~ diffusion coefficient by tortuosity, while V2.1 was not programmed to do so (note: I could have, instead, input a tortuosity = 1 in the FLOW.INP file - same correction)
Results of V2.2 and V2.1 are identical

(4) Run same test problems as on p. 70 item 6 to check chemistry/boiling calculations (equilibrium): boil100, heat_sat1, heat_unsat1 and heat_unsat2. For consistency between the new runs with V2.2 and previous ones with V2.1, I used the same thermo data base (N.S. 20/100) as the one used ~~for~~ previously, but modified the CO_2 record for consistency with the V2.2 version. Also needed to make minor modifications in CHEMICAL.INP and SOLUTE.INP files for consistency with new input formats.
Results of V2.2 and V2.1 are identical for the four problems.

Test problems #2 and 3 in VTR

Location of files

On hydra: users raid/inspycher/react/trea_qa/qa2.2

2phase_flow2.2/*.* } Item (1) above, all i/o files
geothermal2.2/*.* }
heat-pipe2.2/*.* }
aqtrans2.2/*.* Item (2) above, "
gastrans2.2/*.* Item (3) above, "
heat_unsat1/*.* }
heat_unsat2/*.* } Item (4) above, "
heat_sat1/*.* }

The executable is in the .../qa2.2 directory: treactqa2.2, copied from the location given on p 121

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2/18/00 TOUGHREACT V2.2 – QA permeability-porosity-pcap

Objective: check that new coding of porosity-permeability-pcap works fine

Method: run the ~~same~~ similar N.S. 2/18/00 problem as V2.1 qa problem described on p. 71, item 7 and carry out ~~the same~~ N.S. 2/18/00 similar hand checks.

Note: now two methods are used by V2.2 to compute permeability changes from porosity change 1) cubic law (as before) for fractures only and 2) Karman-Cozeny for matrix only. The flag that indicate the rock is matrix, rather than fracture, is porosity < 0.8. Therefore, I ran the problem twice, once with porosity = ~~0.8~~ 0.75 N.S. 02/18/00 and once with porosity = ~~0.999~~ 0.75 N.S. 2/18/00 to check both cases.

Note: because the qa problem setup for V2.1 used porosity of 0.1, and here I raise it to ~~0.8~~ N.S. 2/18/00 0.75, I needed to change the amount (decrease) of heat input in the simulation to keep temperature to a value below 100°C. Also changed the molar volume of dummy calcite in database, liquid saturation to simulate reasonable porosity changes (i.e. not plug everything up). Therefore, this is a different setup than for V2.1 qa.

Test for fractures:

Initial conditions

$T = 25\,^{\circ}C$ N.S. 2/18/00

$\theta = ~~0.8~~$ 0.95

$Sl = ~~0.01~~$ 0.1

$k = 4 \times 10^{-12}\ m^2$

PCFACT (see p. 65) = 1

Note: θ and k now also output in TEC_MIN.DAT file. Checked it there too

Final conditions

$T = ~~89.272~~$ (N.S. 2/18/00) 53.2

$\theta = ~~0.55536~~$ 0.89213

$Sl = ~~0.0099~~$ 0.101

$3.3126\ 10^{-12} \rightarrow k = ~~2.7673\ 10^{-13}~~\ m^2$

PCFACT = ~~0.3122~~ 0.9391

(θ, k, PCFACT read from run_log.dat file with MOPC(13) set to 1)

Hand check using eq (2) on p. 65

$$k_{new} = k\left(\frac{\phi_{new}}{\phi}\right)^3 = 4\cdot10^{-12}\left(\frac{0.89213}{0.95}\right)^3 = 3.3126\ 10^{-12}\ \checkmark$$

$$PCFACT = \left(\frac{k_{new}}{\phi_{new}}\cdot\frac{\phi}{k}\right)^{0.5} = \left(\frac{3.3126\cdot10^{-12}}{4\cdot10^{-12}}\ \frac{0.95}{0.89213}\right)^{0.5} = 0.9391\ \checkmark$$

Checks fine.

Note N.S. 2/18/00 Also check porosity changes: Mineral amount in TEC_MIN.DAT file = 57.87 mol/m³ Mol volume = 1000 mol/dm³ · Mol-Vol · 10⁻⁶ = 57.87 · Mol-Vol · 10⁻³ Mineral vol. frac = 0.05787 · Mol-Vol = 0.05787 Porosity = 1 − 0.05787 = 0.94213

Note N.S. 2/18/00

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Test for matrix

Initial conditions

$T = 25\,°C$

$\phi = 0.75$

$Sl = 0.1$

$K = 1 \times 10^{-12}\ m^2$

$PCFACT = 1$

Final conditions

$T = 41.589$

$\phi = 0.70436$

$Sl = 0.1005$

$K = 2.3694\ 10^{-12}\ m^2$

$PCFACT = 0.7942$

Hand-check using Karman-Cozeny (implemented in V2.2)

$$K_{new} = K \left(\frac{1-\phi}{1-\phi_{new}}\right)^2 \left(\frac{\phi_{new}}{\phi}\right)^3 = 1 \cdot 10^{-12} \left(\frac{1-0.75}{1-0.70436}\right)^2 \left(\frac{0.70436}{0.75}\right)^3$$

$$= 2.3693\ 10^{-12}\ ✓$$

$$PCFACT = \left(\frac{K_{new}}{\phi_{new}} \cdot \frac{\phi}{K}\right)^{0.5} = \left(\frac{2.3694 \cdot 10^{-12}}{1 \cdot 10^{-12}} \cdot \frac{0.75}{0.70436}\right)^{0.5} = 0.7942\ ✓$$

N.S. 3/10/00

checks fine!

> Note added 3/10/00
> ! This formula is in error
> See p. 146. Test was superceded

Location of files

On hydra:
usersraid/nspycher/react/~~qa~~ trea-qa/qa2.2/perm-pcap22/

fracture/ *.* test for fractures, all i/o files
matrix/ *.* test for matrix, all i/o files

Executable: treactq2.2 in the ..../qa.22 folder, copied from location given on p. 121

Note N.S. 2/18/00: also check porosity change. Mineral amount in TEC-MIN.DAT file = 45.64 mol/m³ = 45.64 · mol/vol · 10^{-6} (1000 mol / cc) = 0.04564 vol. fraction
$\phi_{new} = \phi - 0.04564 = 0.75 - 0.04564 = 0.70436$ ✓ (N.S. 2/18/00)

Note N.S. 2/18/00 current test for $\phi < 0.8$ in the code (routine propchs.f) is ~~on~~ PHI(i) < 0.8. Should test be on POR(kimmat) variable instead, in case PHI changes enough to vary from > 0.8 to < 0.8. Fix this in next upgrade. Not a problem here.

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PROJECT NAME Test Problem # 10 in VTR N.S. 3/10/00 N.S. 2/19/00 NOTEBOOK NO.

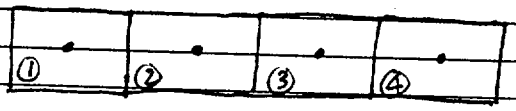
2/19/00 TOUGHREACT QA V2.2 – K thermal variation

Objective: check/verify the new option to allow changing thermal conductivities with time. With this option, factors changing with time are input into the GENER block and the input thermal conductivities in the ROCKS block are multiplied by these factors. N.S. 2/19/00

Method: set up a simple thermal run and hand calculate the thermal conductivities from input factors and conductivities. Set the input flag MOP(3) to 6 to allow printout of thermal conductivities (variable name CON) in the main output file.

Problem setup: 4 blocks, 1-D horizontal, same properties

Tinit 90°C 25 25 25 °C



N.S. 2/19/00 K thermal max 1000 1000 1000 1000

same k factors changing with time (see below)
not changing with time

With this setup, K thermal at connection ①-② remains constant at 1000 W/m C, and the variable K thermal (K effective) at connection ③-④ should be factor x 1000.

```
GENER
A11 3
                                HEAT 0.0000e+00                          5
      0.0E+00  5.000000E+00  1.000000E+01  1.500000E+01 } times
 2.000001E+01
        1.000         0.500         0.250         0.100 } factors
        0.010
A11 4
                                HEAT 0.0000e+00                          5
      0.0E+00  5.000000E+00  1.000000E+01  1.500000E+01 } times
 2.000001E+01
        1.000         0.500         0.250         0.100 } factors
        0.010
```

Run for 20 seconds with Δt = 1 sec.

Results:

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TOUGHREACT V2.2 qualification
Hand check effective thermal conductivities changing with time (Keff)

Time (s)	kfact	Intepolated kfact	Kmax (W/m C)	Hand Calc. Keff (W/m C)	TOUGHREACT Keff * (W/m C)
0	1	1	1000	1000	1000
1		0.9	1000	900	900
2		0.8	1000	800	800
3		0.7	1000	700	700
4		0.6	1000	600	600
5	0.5	0.5	1000	500	500
6		0.45	1000	450	450
7		0.4	1000	400	400
8		0.35	1000	350	350
9		0.3	1000	300	300
10	0.25	0.25	1000	250	250
11		0.22	1000	220	220
12		0.19	1000	190	190
13		0.16	1000	160	160
14		0.13	1000	130	130
15	0.1	0.1	1000	100	100
16		0.082	1000	82	82
17		0.064	1000	64	64
18		0.046	1000	46	46
19		0.028	1000	28	28
20 **	0.01	0.01	1000	10	10

* As read in main output file; variable CONI, after setting MOP(3)=6 to print this variable
** Last time step is 20.00001. Needs to be slighly > 20 for last Keff to be calculated properly

SUPERCEDED Minor bug was fixed. See p. 147 N.S. 3/10/00

Note: found minor bug to be corrected in future upgrades. If last time in the GENER (here = 20 sec) is not set slightly larger, Kmax is not multiplied by the factor for the last time step (i.e. here we would have Keff at 20 sec = 1000 w/m c).

As shown in table above, hand-calculated Keff match those output by the program.

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Location of test files

On hydra: users/raid/react/trec_qc/qa2.2/k_thermal2.2

check_kTh.xls above table
FLOW.INP, FLOW.OUT input & output files

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PROJECT NAME N.S. 3/10/00 Test Problem # 8 in √TR NOTEBOOK NO.

3/1/00

TOUGHREACT QA - Gas diffusion coefficient

Objective: check/verify new option for calculating gas diffusion coefficients as function of P and T, and use of tortuosity from the "Rocks" input block for weighting diffusivity.

Method: run the gas transport test (p. 128, item # same as RUNS on p. 60 and 61) setting the gas diffusion coefficient in SOLUTE.INP equal to -1 which is the flag to enable calculation of diffusion coefficients for gases as function of T, P, and tortuosity. Compare the result of TOUGHREACT N.S. 3/1/00 with the analytical solution (see p. 60) N.S. 3/1/00 and using a hand-calculated diffusion coefficient N.S. 3/1/00 with the hand-calculated with the equation implemented into toughreact V2.

$$D = \frac{RT}{3\sqrt{2}\,\pi P N_a d^2}\sqrt{\frac{8RT}{\pi M_w}} \qquad (1)$$

D diffusion coeff in m^2/s
R gas constant 8.314 $m^2\,kg\,s^{-2}\,mol^{-1}\,K^{-1}$
T temperature in °K
π 3.1416
P pressure (Pa = $kg\,m^{-1}\,s^{-2}$)
N_a Avogadro's number 6.0221×10^{23} mol^{-1}
d molecular diameter = 2.5×10^{-10} m for CO_2
M_w = molecular weight (kg/mol) = 0.04401 for CO_2

(From Lasaga, 1998, "Kinetic Theory in the Earth Sciences", Princeton, N.J., p. 322)

Results

Hand calculate D from equation 1 above:

T = 35 °C
P = 0.998 Pa (at x = 1m) } problem setup (see p. 57)

D = 1.97×10^{-5} m^2/s (using eq 1)

Effective D = D x tortuosity (0.2 (set in FLOW.INP file))

Deff = $1.97 \times 10^{-5} \times 0.2 \times 60 \times 60 \times 24$ = 3.4045×10^{-1} m^2/day (conversion to m^2/day)

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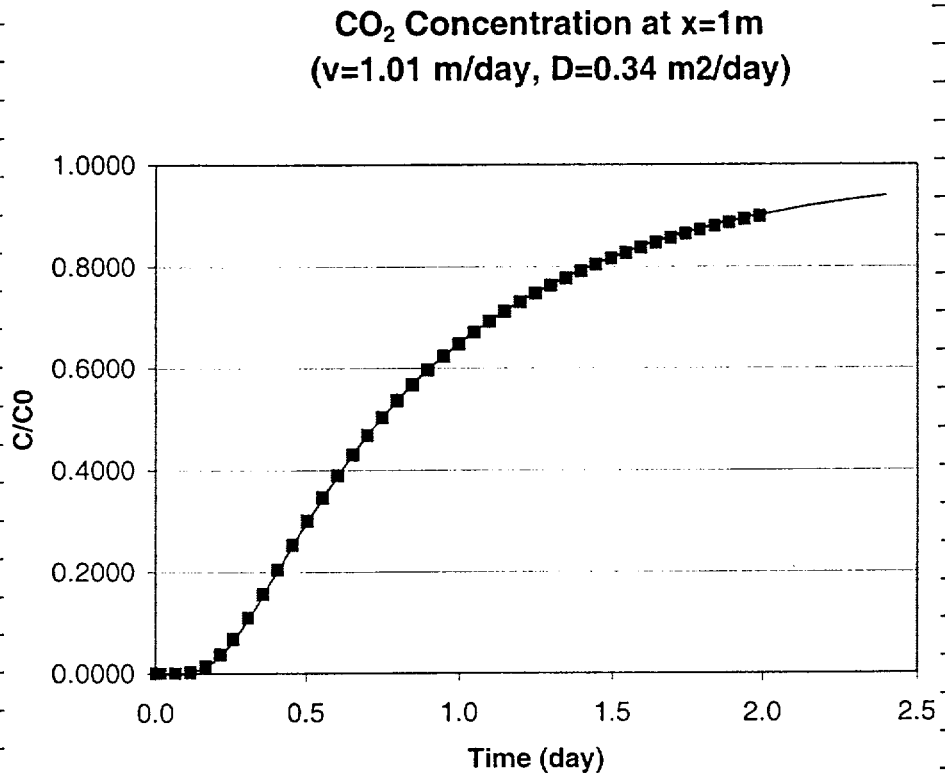
Using Deff above and analytical solution on p. 60 (set D=Deff in this equation), then plotting results and comparing to toughreact V 2.2 solution, we get good match as shown below:



Symbols: TOUGHREACT (version 2.2) — from TIME.DAT output file
Solid Lines: Analytical Solution (Ogata and Banks, 1961) — see p. 60

Note: this problem was run with database thermoh2o_nrs 3/10/00 solthymp2.06.dat (same as thermoh2o_nrs 3/10/00 solthymp2.05.dat (see p 111) but with CO2 molecular weight in kg/mol instead of g/mol).

Location of files: on hydra

usersraid/mspycher/react/trea_qa/qa2.2/gas-diffus/2.2/
check_diff.xls (above plot and calcs)
FLOW.INP, SOLUTE.INP, CHEMICAL.INP } input files
solthymp2.06.dat
TIME.DAT output plotted above

executable: treactq2.2 (see p. 121 for location)

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PROJECT NAME N.S. 3/1/00 N-> 3/10/00 TEST Problem # 11 in VTR NOTEBOOK NO.

3/1/00 TOUGHREACT V2.2 QA: gas & mineral volume fraction printout

Objective: check/verify option that allows outputting gas and mineral volume fraction in TECPLOT files (as opposed to gas pressures) and mineral moles per volume medium, which is the original option.

Method: run test case heat_unsat1 (p. 129, item # 1) with option to output minerals and gas N.S. 3/1/00 volume fractions (by setting new flag "minflag" =1 in SOLUTE.INP file). Then check results against the original run output (in bars and mol/m^3) and converting the units by hand:

$$V_{fraction} = \frac{mol}{m^3} \cdot mv \cdot \frac{1}{1{,}000{,}000}$$

(molecular volume in cm^3/mol)

$$\left.\begin{aligned} P_i V &= n_i RT \\ P v_i &= n_i RT \end{aligned}\right\} \Rightarrow \frac{v_i}{V} = \frac{P_i}{P} \Rightarrow V_{fraction} = \frac{P_i}{P}$$

(for ideal gas / perfect mixture)

P_i = partial pressure
P = total pressure
V = total volume
v_i = "partial" volume of pure i

con't 3/2/00 Results: conversions were checked to be correct.

Location of files: on hydra

/users/esid/nspychner/react/trea_qa/qa2.2/

gas_min_conver2.2/*.* run with minflag = 1 (output in vol. fraction)
check_conver.xls checking spreadsheet

heat_unsat1_2.2/*.* run with minflag = 0 (original output in bars and N.S. 3/2/00 mol/m^3)

N.S. 3/2/00
executable: /trea treact q2.2 (see p 121 for location)

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PROJECT NAME N.S. 3/10/00 Test Problem # 6 in VIR — NOTEBOOK NO.

3/6/00

TOUGHREACT V2.2 QA : reaction rates

Objectives: check/verify new options that affect reaction rates, as follows:
- new rate law option: nplaw = 1
- new surface areas options
  - imflg = 1 for inputting areas in m^2/m^3 active fracture model

Also check that options in existing prior version were not affected

Method: run a simple problem and hand calculate reaction rates given various input options for calculation surface areas and rate laws.

Summary of surface area and rate law options

(See TOUGHREACT V2.1 QA manual LBNL-report 44846 and AMR U0110 - Drift Scale Coupled Processes, and also E. Sonnenthal notebook for more details)

- Surface area - existing option (imflg = 0)

$$A_e = A \times \frac{mw}{mv} \times 0.1 \times \frac{Vf}{mv}(1-\phi) \times \frac{mv}{\rho w \cdot \phi \cdot Sl} \times Sl$$

(mw: g/mol; A: cm^2/g; mv: l/mol; Vf: $m^3_{mineral}/m^3$; pre (mineral): mol/l medium; ρw: 1000 Kg/m^3; Ae: m^2/Kg H2O)

"pre(i)" is a toughreact variable

Ae effective surface area (m^2/Kg H2O)
Sl liquid saturation
A input surface area in cm^2/g
mw molec weight (g/mol)
mv molar volume (mol/l)
Vf input mineral volume fraction $\frac{V_{min}}{V_{solid}}$
ϕ porosity
ρw water density in kg/m^3

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- Surface area - new option (imflg = 1)

$$Ae = A \times \frac{Vf}{mv}(1-\phi) \times \frac{mv}{\rho_w \cdot \phi \cdot sl} \times sl = \frac{A \times Vf(1-\phi)}{\rho_w \phi}$$

Ae: m^2 / kg_{H2O}; A: $m^2/m^3_{mineral}$; $\frac{Vf}{mv}(1-\phi)$: pre (mineral) $\frac{mol}{l_{medium}}$

Variables same as previous except input A in m^2/m^3

- Surface area - new option if active-fracture model is enabled (afm ≠ 1.)

$$afm = [(sl - slmin)/(1 - slmin)]^{1+\gamma}$$

(set afm = 1.0 if this model is not enabled)

If imflg = 0 we get

$$Ae = A \times \frac{mw}{mv} \times 0.1 \times \frac{Vf}{mv}(1-\phi) \times \frac{mv}{\rho_w \cdot \phi \cdot sl} \times afm$$

A: cm^2/g → m^2/m^3; $\frac{Vf}{mv}(1-\phi)$: pre mol/l_{medium}

If imflg = 1 we get

$$Ae = A \times \frac{Vf}{mv}(1-\phi) \times \frac{mv}{\rho_w \cdot \phi \cdot sl} \times afm$$

A: m^2/m^3; $\frac{mv}{\rho_w \cdot \phi \cdot sl}$: pre

- Rate law - existing option (nplaw = 0)

n.s. 3/6/00 [t̄ Δt]

$$Rate^{[t]} = K \cdot Ae \left[(Q/K)^m_{[t]} - 1\right]^n \times \text{sign of } \log(Q/K)$$

Rate: $mol/kg \cdot s$

m and n = 1

K is rate constant $= K_o \exp\left[\frac{-EA}{R}\left(\frac{1}{T_K} - \frac{1}{298.15}\right)\right]$

K_o: $mol/kg \cdot s$ = K at 25°C

T_K = temp in °K

EA = activation energy (kJ/mol)

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R = constant = 0.008314 (kJ/mol·°K)
Q/K saturation index (saturated > 1; undersat < 1)

- New rate law (precipitation only) N.S. 3/6/00

$$\text{Rate}_{[t]} = k \cdot A_e^{[t-\Delta t]} \left(\frac{Q}{K}\right)_{[t]}^{n} \underbrace{\left(1 - 1/\left[\left(\frac{Q}{K}\right)_{[t]}^{n}\right]^2\right)}$$

[t] means at t
[t-Δt] means previous t step
(added so that Rate → 0 when Q/K → 1)

Test problem setup

Use two grid blocks: 1 fracture and 1 matrix
Use two minerals: calcite nplaw = 0 imflg = 0
am. silica nplaw = 1 imflg = 1
(set in each grid block)

Turn on the active-fracture model for fracture block
Use constant Δt steps of 200 seconds over a 1000 seconds time span (arbitrary)
Use initial liquid saturations that remain ~ constant ~~(after running the problem for T >> 1000s)~~ N.S. 3/6/00
~~(determined by running this setup over to~~
(determined after running an initial simulation with a large total simulation time >> 1000 s.)
Use totally arbitrary other input parameters and rate constants to yield a noticeable variation in log(Q/K) over the time frame considered (supersaturated system approaching equilib.)

Calculate by hand (spreadsheet, next page) the amount of precipitating minerals at each time step using the formulas above, and compare with TOUGHREACT results:

$$\text{amount}_{[t]} = \text{rate}_{[t]} \times \Delta t$$

(Δt = 200 s in this case)

The difference between the hand-calculated amount should be less than 1% N.S. 3/6/00 (and TOUGHREACT V2.2 output)

Results: The two forms of rate laws and three forms of surface area calculations were verified to be correctly implemented into

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TOUGHREACT V2.2. As shown in the spreadsheets below, differences between hand-calculated and TOUGHREACT-calculated mineral amounts are ≤ 1%

Effective Surface Area (S) in matrix (without active-fracture model)
If input flag imflg=0 (set for calcite): (1 − ϕ) N·S. 3/6/00
S = [A * mw/mv * Vf * (phi) / (Sl*phi*rhow) * 0.1] * Sl (eq.3-4 in thoughreact v2.1 QA manual)
with A in cm2/g_min and rhow=1000 kg/m3

If input flag imflg=1 (set'for am. silica):
S = A * Vf * (1-phi)/ (Sl*rhow*phi) * Sl (new option in v2.2)
with A in m2/m3_min and rhow=1000 kg/m3

Rate Laws
Rate constant k = k0 * exp (EA/R * (1/Tk-1/298.15)

If flag nplaw=1 (set for am. silica):
rate = k * S * [(Q/K)**n - 1/((Q/K)**(n*2))]
Note: the second (Q/K) term is added so the rate trends to zero as Q/K approaches 1

If flag nplaw=0 (set for calcite):
rate = k * S * [(Q/K) - 1]

AMORPHOUS SILICA in MATRIX (grid block m_0_1)
New rate law, and A in m2/m3_min

Input data (arbitrary!)	
temp T (C)	45
liq.saturation, Sl	0.2596
porosity, phi	0.11
vol.fraction, Vf	0.1
mol.vol., mv (l/mol)	0.029
molec.wt, mw (g/mol)	60.084
surf.arera, A (m2/m3)	100
ko (mol/kg_h2o/s)	1.00E-05
exponent n	4.40E+00
EA (kJ/mol)	62.8
R (kJ/mol/K)	0.008314

Calculate k and starting S	
S (m2/kg_h2o)	0.080909
k (mol/kg_h2o/s)	4.92E-05

Calculated by TOUGHREACT (from file chdump.dat)		
time (s)	amount (mol/kg_h2o)	log(Q/K)
0	0.0000E+00	0.5837
200	6.80E-03	0.211943
400	1.40E-03	0.068636
600	3.95E-04	0.017652
800	9.75E-05	0.004114
1000	2.26E-05	0.000937

"Hand"-calculated	
Eff.Area S (m2/kg_h2o)	amount (mol/kg_h2o)
8.09091E-02	
8.09288E-02	6.8002E-03
8.09329E-02	1.3970E-03
8.09340E-02	3.9513E-04
8.09343E-02	9.7519E-05
8.09344E-02	2.2557E-05

Check amount difference (%)
0.0007
0.0209
0.0205
0.0150
-0.0034

Note: S at (t>0) is calculated here as:
S at (t-dt) + amount * mol.volume * surf_area(m2/m3) * 1e-3

CALCITE in MATRIX (grid block m_0_1)
Original rate law, and A in cm2/g

Input data (arbitrary!)	
temp T (C)	45
liq.saturation, Sl	0.2596
porosity, phi	0.11
vol.fraction, Vf	0.1
mol.vol., mv (l/mol)	0.036934
molec.wt, mw (g/mol)	100.087
surf.arera, A (cm2/g)	200
ko (mol/kg_h2o/s)	1.00E-08
EA (kJ/mol)	41.87
R (kJ/mol/K)	0.008314

Calculate k and starting S	
S (m2/kg_h2o)	43.85091
k (mol/kg_h2o/s)	2.89E-08

Calculated by TOUGHREACT (from file chdump.dat)		
time (s)	amount (mol/kg_h2o)	log(Q/K)
0	0.0000E+00	0.8863
200	3.15E-04	0.350817
400	1.01E-04	0.145453
600	4.09E-05	0.064986
800	1.81E-05	0.029897
1000	8.27E-06	0.01393

"Hand"-calculated	
Eff.Area S (m2/kg_h2o)	amount (mol/kg_h2o)
4.38509E+01	
4.38515E+01	3.1520E-04
4.38517E+01	1.0089E-04
4.38518E+01	4.0934E-05
4.38519E+01	1.8073E-05
4.38519E+01	8.2661E-06

Check amount difference (%)
0.0004
-0.0023
0.0017
0.0045
-0.0004

Note: S at (t>0) is calculated here as:
S at (t-dt) + amount * mol.weight * surf_area(cm2/g) * 1e-4

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Effective Surface Area (S) for fractures (using active-fracture model)
afm = [(Sl-Smin)/(1-Smin)] ** (1+ gamma)

If input flag imflg=0 (set for calcite): 4pi (1 - phi) N.S. 3/6/00
S = [A * mw/mv * Vf * ~~(phi-1)~~ / (Sl*phi*rhow) * 0.1] * afm (eq.3-4 in thoughreact v2.1 QA manual * afm / Sl)
with A in cm2/g_min and rhow=1000 kg/m3

If input flag imflg=1 (set for am. silica):
S = A * Vf * (1-phi)/ (Sl*rhow*phi) * afm (new option in v2.2)
with A in m2/m3_min and rhow=1000 kg/m3

Rate Laws
Rate constant k = k0 * exp (EA/R * (1/Tk-1/298.15)

If flag nplaw=1 (set for am. silica):
rate = k * S * [(Q/K)**n - 1/((Q/K)**(n*2))]
Note: the second (Q/K) term is added so the rate trends to zero as Q/K approaches 1

If flag nplaw=0 (set for calcite):
rate = k * S * [(Q/K) - 1]

AMORPHOUS SILICA in FRACTURE (grid block f_0_1)
New rate law, and A in m2/m3_min

Input data (arbitrary!)	
temp T (C)	45
liq.saturation, Sl	0.1415
porosity, phi	0.11
vol.fraction, Vf	0.1
mol.vol., mv (cc/mol)	0.029
molec.wt, mw (g/mol)	60.084
surf.arera, A (m2/m3)	100
gamma	0.4095
minimum Sl, Smin	1.00E-04
ko (mol/kg_h2o/s)	1.00E-05
exponent n	4.40E+00
EA (kJ/mol)	62.8
R (kJ/mol/K)	0.0083143

Calculate k and starting S	
S (m2/kg_h2o)	0.0362961
k (mol/kg_h2o/s)	4.92E-05

Calculated by TOUGHREACT (from file chdump.dat)		
time (s)	amount (mol/kg_h2o)	log(Q/K)
0	0.0000E+00	0.5837
200	5.98E-03	0.278167
400	1.53E-03	0.145091
600	6.59E-04	0.072152
800	3.13E-04	0.032657
1000	1.40E-04	0.01374

"Hand"-calculated	
Eff.Area S (m2/kg_h2o)	amount (mol/kg_h2o)
3.62961E-02	
3.63135E-02	5.9755E-03
3.63179E-02	1.5340E-03
3.63198E-02	6.5899E-04
3.63207E-02	3.1291E-04
3.63212E-02	1.4013E-04

Check amount difference (%)
-0.0018
0.0526
0.0696
0.0831
0.0915

Note: S at (t>0) is calculated here as:
S at (t-dt) + amount * mol.volume * surf_area(m2/m3) * 1e-3

CALCITE in FRACTURES (grid block f_0_1)
Original rate law, and A in cm2/g

Input data (arbitrary!)	
temp T (C)	45
liq.saturation, Sl	0.1415
porosity, phi	0.11
vol.fraction, Vf	0.1
mol.vol., mv (cc/mol)	0.036934
molec.wt, mw (g/mol)	100.087
surf.arera, A (cm2/g)	200
gamma	0.4095
minimum Sl, Smin	1.00E-04
ko (mol/kg_h2o/s)	1.00E-08
EA (kJ/mol)	41.87
R (kJ/mol/K)	0.0083143

Calculate k and starting S	
S (m2/kg_h2o)	19.671699
k (mol/kg_h2o/s)	2.89E-08

Calculated by TOUGHREACT (from file chdump.dat)		
time (s)	amount (mol/kg_h2o)	log(Q/K)
0	0.0000E+00	0.8863
200	2.45E-04	0.499221
400	1.04E-04	0.281889
600	5.46E-05	0.170332
800	3.18E-05	0.107013
1000	1.95E-05	0.068696

"Hand"-calculated	
Eff.Area S (m2/kg_h2o)	amount (mol/kg_h2o)
1.96717E+01	
1.96722E+01	2.4534E-04
1.96724E+01	1.0396E-04
1.96725E+01	5.4636E-05
1.96726E+01	3.1789E-05
1.96726E+01	1.9497E-05

Check amount difference (%)
-0.0028
0.0055
0.0157
0.0252
0.0312

Note: S at (t>0) is calculated here as:
S at (t-dt) + amount * mol.weight * surf_area(cm2/g) * 1e-4

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Location of files: on hydra

/users/raid/nspycher/react/trea_qa/qa2.2/reac_rates/2.2/1

chk_rates.xls spreadsheet shown on p. 140-141
all other standard input/output files
(e.g. CHEMICAL.INP, FLOW.INP, SOLUTE.INP, FLOW.OUT, chdump.dat, etc. etc.)

N.S. 3/6/00
~~Exect~~
Executable: treactqa2.2 (see p. 121 for location)

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PROJECT NAME TEST PROBLEM # 5 in VTR N.S. 3/19/00 NOTEBOOK NO.

3/9/00 TOUGHREACT QA – test against eos3 V1.4 – Thermal

This is an add-on to the entry on p. 120 to 123, with same objective, methods, and acceptance criteria. I ran a different problem as the one described on p. 120, to provide additional comparison of TOUGHREACT V2.2 against EOS3 V1.4 for a thermal problem that involves dryout (to better test the capillary pressure extrapolation at low saturations)

Problem setup: Similar to problem on p. 120, but impose a thermal load for 10 years. Use the drift-scale model used for AMR U0110 (YMP-LBNL-DSM-NS-1, p. 36, item 2), but run for only 10 years and delete the thermal conductivity factors in the GENER files because these are not implemented into EOS3 V1.4.

Results: are shown on the next pages. Both codes yield results within the acceptance criteria of 1%

location of test files (excepts printouts on p. 144 N.S. 3/9/00 corr.)

on calx /nspycher/ treactq 2.2 – qa/

qa2.2_vs_eos3_V1.4/
eos3_V1.4/ *.* eos3 I/O files
treactq 2.2/ *.* treact I/O files
compare.xls compare results (p. 145)

Source codes: see p. 121

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Results of TOUGH2 EOS3 V1.4

```
F   2
 0.8857198956136E+05 0.1099252404033E+02 0.8252401221500E+02 0.7475959668559E-02 0.74759596
M   2
 0.8916011893525E+05 0.1000665063026E+02 0.8252568309643E+02 0.9933493697381E+00 0.99334936
F   3
 0.8857116366438E+05 0.1097637937473E+02 0.8029490061670E+02 0.2362062526820E-01 0.23620625
M   3
 0.8856187566477E+05 0.1000589434041E+02 0.8029469743783E+02 0.9941056595891E+00 0.99410565
F 300
 0.8862635183358E+05 0.1096099869683E+02 0.5140137531991E+02 0.3900130317217E-01 0.39001303
M 300
 0.8862746453710E+05 0.1000391008293E+02 0.5140137280144E+02 0.9960899170656E+00 0.99608991
F 302
 0.8857414334037E+05 0.6458583803306E+00 0.7910770232097E+02 0.0000000000000E+00 0.00000000
M 302
 0.9798394895541E+05 0.1001280164361E+02 0.7910750778802E+02 0.9871983563892E+00 0.98719835
F1106
 0.9125011671062E+05 0.1083708744742E+02 0.2960376083654E+02 0.1629125525800E+00 0.16291255
M1106
 0.9125382488760E+05 0.1000956089049E+02 0.2960380670553E+02 0.9904391095118E+00 0.99043910
F1107
 0.9167147381815E+05 0.1083712735736E+02 0.3090478066708E+02 0.1628726426371E+00 0.16287264
M1107
 0.9170377931300E+05 0.1000772614983E+02 0.3090482994126E+02 0.9922738501719E+00 0.99227385
dr  2
 0.1079710342356E+06 0.1000000000000E+01 0.8916961488880E+02 0.0000000000000E+00 0.00000000
dr  3
 0.1076640198905E+06 0.1000000000000E+01 0.8813936330273E+02 0.0000000000000E+00 0.00000000
```

Results of TOUGHREACT V2.2

```
F   2           0.99000000E+00 0.27570000E-12 0.27570000E-12 0.27570000E-12
 0.8857202554025E+05 0.1099267993559E+02 0.8255515925758E+02
M   2           0.11000000E+00 0.40700000E-17 0.40700000E-17 0.40700000E-17
 0.8916197023364E+05 0.1000663696971E+02 0.8255683994723E+02
F   3           0.99000000E+00 0.27570000E-12 0.27570000E-12 0.27570000E-12
 0.8857118862612E+05 0.1097640356178E+02 0.8031921662638E+02
M   3           0.11000000E+00 0.40700000E-17 0.40700000E-17 0.40700000E-17

F 300           0.99000000E+00 0.27570000E-12 0.27570000E-12 0.27570000E-12
 0.8862635594992E+05 0.1096099814095E+02 0.5140061113282E+02
M 300           0.11000000E+00 0.40700000E-17 0.40700000E-17 0.40700000E-17
 0.8862746391857E+05 0.1000391266871E+02 0.5140060861418E+02
F 302           0.99000000E+00 0.27570000E-12 0.27570000E-12 0.27570000E-12
 0.8857415891780E+05 0.6455710377740E+00 0.7912869319296E+02
M 302           0.11000000E+00 0.40700000E-17 0.40700000E-17 0.40700000E-17
 0.9800246599962E+05 0.1001279612395E+02 0.7912849803592E+02

F1106           0.99000000E+00 0.31230000E-13 0.31230000E-13 0.31230000E-13
 0.9125011970578E+05 0.1083708749693E+02 0.2960376082468E+02
M1106           0.33100000E+00 0.60690000E-17 0.60690000E-17 0.60690000E-17
 0.9125382499431E+05 0.1000956089048E+02 0.2960380669357E+02
F1107           0.99000000E+00 0.31230000E-13 0.31230000E-13 0.31230000E-13
 0.9167147679203E+05 0.1083712739312E+02 0.3090478065515E+02
M1107           0.33100000E+00 0.60690000E-17 0.60690000E-17 0.60690000E-17
 0.9170377945284E+05 0.1000772614982E+02 0.3090482992924E+02

dr  2           0.10000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.1079872748189E+06 0.1000000000000E+01 0.8922411395616E+02
dr  3           0.10000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.1076791801409E+06 0.1000000000000E+01 0.8819023681979E+02
```

compare - see % difference on p. 145

etc

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475959668559E-02
·93 3697381E+00
.362062526820E-01
·941056595891E+00

:900130317217E-01
·960899170656E+00
)000000000000E+00
)871983563892E+00

.629125525800E+00
)904391095118E+00
.628726426371E+00
)922738501719E+00

)000000000000E+00
)000000000000E+00

Comparison between TOUGHREACT V2.2 and EOS3 V1.4

Grid Block	P difference %	Sg difference %	T difference %
F 2	0.0000	-0.0377	-0.0157
M 2	-0.0021	-0.0378	0.2054
F 3	0.0000	-0.0303	-0.0025
M 3	0.0000	-0.0303	0.2088
F 300	0.0000	0.0015	0.0001
M 300	0.0000	0.0015	-0.0661
F 302	0.0000	-0.0265	0.0445
M 302	-0.0189	-0.0265	0.0431
F1106	0.0000	0.0000	0.0000
M1106	0.0000	0.0000	0.0000
F1107	0.0000	0.0000	0.0000
M1107	0.0000	0.0000	0.0000
dr 2	-0.0150	-0.0611	0.0000
dr 2	-0.0141	-0.0577	0.0000

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3/10/00 TOUGHREACT V2.2 QA - Pcap - Permeability porosity correction + minor fixes and re - QA

Objective: report error found in the formula used previously to couple capillary pressure to permeability and porosity changes, implement the correct formula into the code, QA the results, and also implement minor fixes and re-QA

Correction:

The formula for calculating P_c' on p. 65 was found in error. The correct formula should be:

$$P_c' = P_c \times \frac{(k/\phi)^{0.5}}{(k'/\phi')^{0.5}} \quad (1)$$ (reverse of what it was previously)

(P_c', k', and ϕ' are new values of cap pressure, permeability and porosity, respectively. P_c, k, and ϕ are the original values. See p. 65)

This was corrected in the code (V2.2) prior to QA release. Implications to THC simulations so far are insignificant because the calculated porosity changes in all our THC simulations, so far, applying to Yucca Mountain, have been very small.

QA of correction (VTR Test Problem # 7)

The test described on p.130-131 was run again with the corrected version of V2.2. The new value of PCFACT (see p.131) should be:

$$PCFACT = \left(\frac{\phi_{new}}{k_{new}} \cdot \frac{k}{\phi}\right)^{0.5} \quad (2)$$

test for fractures: PCFACT from TOUGHREACT (from run.log.dat file) = 1.064865

Hand calc. from (2) $\sqrt{\frac{.89213}{3.3126\,10^{-12}} \cdot \frac{4.10^{-12}}{0.95}} = 1.06487$ ✓

test for matrix: PCFACT from TOUGHREACT = 1.25916

Hand calc. from (2) $\sqrt{\frac{.70436}{2.3694\,10^{-12}} \cdot \frac{4.10^{-21}}{0.75}} = 1.2591$

ϕ and k values are the same as previously

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other minor fixes

1) Fix diffusion coefficient calculation for gases so that the gas molecular weight can be input in g/mol [instead of kg/mol].

QA by running again the test on p. 134-135 using the original database ~~N-S 3/10/99 softhyimp~~ thermokapps2.05 with CO_2 mol weight in g/mol. Results are identical to those shown on p. 135.

2) Fix minor bug with thermal conductivity factors that was brought up on p. 133. Rerun the same QA test problem as on p. 132-133, with last time step = 20.00 s. Results are identical to those shown on p. 133.

3) Fix an insignificant potential problem with the test for porosity < 0.8 for permeability-porosity coupling calculations (p. 130). Changed the test to use the original porosity variable (POR) rather than the updated variable (PHI) for this test. Does not affect runs to date with matrix porosity $<< 0.8$. QA'd again this option by running the test on p. 130. Get exact same results of ϕ and k as previously.

Total Re-QA of V2.2

For peace of mind, all other QA tests (p. 120 to 145) were ran again with the new executable code, and produced the same results for each tests as with the previous executable without fixes.

File locations: no changes from those described on p. 120 to 145

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Convergence is reached between 2 and 12 sequential iterations. The difference in results between V 1.0, 2.1, and 2.1 with sequential iteration is 'shown' on the table below

Note added 4/29/99: ~~reaction(s)~~ N.S. 4/29/99 surface area(s) in m²/kg H2O in version 1.0 were calculated for a water density of 0.81 at 240°C. The surface area(s) in version 2.1 are in cm²/g from original source (Johnson et al., 1998). For better comparison between both runs, rerun 2.1 with surface areas divided by 0.81 (not saved run), with results shown handwritten in adjacent table.

Yucca Mountain Project WBS 1.2.3.14.2
QA of treactq2.1 - modeling of tuff dissolution experiment PFR-5 of Johnson et al. (1998)
(Sample problem 2 of TOUGHREACT V 1.0 Q version)
By: N.S. 5/5/99

see notes in margin

Comparison of modeling results at 35.96 days, grid block rk53 (outlet)
(versions 1.0 versus 2.1 without sequentiual iteration, and versus 2.1 with chem/transport sequential iterations)

	V 1.0 (mol/l)	V 2.1 (mol/l)	V 2.1** (mol/l)	V 1.0 (mg/l)	V 2.1 (mg/l)	V 2.1* (mg/l)	Measured** (ppm)	Mol.weight g/mol
Ca	3.00E-06	5.35E-07	4.79E-07	0.120	0.021 (.023)	0.019	0.084	40.08
Na	8.58E-04	4.65E-04	4.45E-04	19.71	10.69 (10.2)	10.23	14.91	22.99
Si	1.08E-02	9.81E-03	9.79E-03	302.5	275.6 (276)	274.8	353.0	28.09
K	5.59E-05	3.04E-05	2.91E-05	2.185	1.190 (1.19)	1.139	2.402	39.10
Al	8.62E-05	1.86E-04	1.95E-04	2.325	5.021 (4.5)	5.253	7.540	26.98
pH	7.643	7.240	7.197				NA	
	(mol/m3)	(mol/m3)	(mol/m3)	(vol %)	(vol %)	(vol %)		Mol.volume cm3/mol
kaolinite	0.00E+00	1.11E-05	3.64E-09	0.0000	0.0000	0.0000	NA	99
paragonite	0.00E+00	1.39E-10	2.80E-55	0.0000	0.0000	0.0000	NA	132.53
muscovite	0.00E+00	2.74E-11	7.75E-24	0.0000	0.0000	0.0000	NA	140.71
gibbsite	0.00E+00	8.78E-10	3.59E-40	0.0000	0.0000	0.0000	NA	31.9
pyrophyllite	0.00E+00	1.01E+00	1.43E-04	0.0000	0.0000	0.0000	NA	126.6
boehmite	3.39E-18	6.74E-10	1.86E-22	0.0000	0.0127 (.0092)	0.0000	NA	19.535
diaspore	0.00E+00	1.96E-09	3.97E-21	0.0000	0.0000	0.0000	NA	17.7
k-feldspar	2.75E-01	6.34E-01	8.38E-01	0.0030	0.0068 (.0041)	0.0090	NA	108
albite-low	4.05E+00	9.54E+00	1.18E+01	0.0405	0.0955 (.0969)	0.1184	NA	100.07
anorthite	-1.07E-02	-2.59E-03	8.63E-03	-0.0001	0.0000 (.0397)	0.0001	NA	100.79
quartz	-1.59E-01	-1.31E-01	-1.23E-01	-0.0004	-0.0003 (.00)	-0.0003	NA	22.688
cristobalite	-1.22E+02	-2.45E+02	-2.46E+02	-0.3125	-0.6284 (.4772)	-0.6309	NA	25.7
total vol % >				-0.2695	-0.5136	-0.5037	NA	

(V 2.1 column circled)* disgard 5/24/99 N.S. superceeded see p. 82

* Sequential iterations between chemistry and transport → N.S.
** Table 2 of Johnson et al., 1998, at t=35.96 days

corrected 5/10/99. see case (12) on p. 77

Original porosity (%) = 42.5
H2O density is 0.813 g/cm3 at 240 C
However, toughreact assumes density = 1 g/cm3, so here we assume the same and thus assume mg/l=ppm

[signature] cont
4/29/99

(6) Run same test problems used to check ~~compute~~ N.S. 4/29/99 chemistry calculation with TOUGHREACT V 1.0 (NS-1, p 125 to 131). These tests are: boil100, heat_sat1, heat_unsat1 and heat_unsat2)

Boil100: results of V1.0 and treactq2.1 are identical

Heat_sat1: same as above

heat_unsat1: same as above except at one time step albite-low amounts are different by ~~0.0004~~ N.S. 4/29/99 less than 0.03% — very small, considered to be the result of roundoff due to the different data formulation in CHEMICAL.INP file between V.1.0 and 2.1

Heat_unsat2: identical results between V 1.0 and 2.1

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Note: this [illegible]

7) Test run for permeability & capillary pressure changes due to changing porosity.
This is a simplified run with following set up:
2 grid blocks with initial porosity = 0.1
1 time step with heat input to raise water temp
1 dummy calcite mineral with artificially increased molar volume to result in large porosity decrease upon precipitation

Initial Conditions		Final conditions
$T =$	25 °C	76.551
$\phi =$	0.1	0.06942
$S_l =$	0.01	0.01
$K =$	4 E-12 m^2	.13384 E-11
PCFACT (see p.65)	1	0.6942

from SAVE and run_log.dat files
(the latter contains porosity, permeability and pcfact data if MOP(23) is set=1)

Note: this formula in error. This test was superseded. See p. 146 N.S. 3/10/00

Hand check using eq (2) on p. 65

$$k' = 4 \cdot 10^{-12} \left(\frac{0.06942}{0.1}\right)^3 = 0.1338 \; 10^{-11} \checkmark$$

(0.1 crossed out, N.S. 4/29/99)

$$\text{PCFACT} = \sqrt{\frac{k'}{\phi'} \cdot \frac{\phi}{k}} = \sqrt{\frac{0.1338 \; 10^{-11}}{0.06942} \cdot \frac{0.1}{4 \cdot 10^{-12}}} = 0.6942 \checkmark$$

I also checked that the PCFACT parameters are passed to routine PCAP correctly by printing this factor from routine PCAP.

(8) Aqueous transport: run the same transport test as for the qualification of TOUGHREACT V1.0 (problem 4 in QA manual), for comparison with T2R3D results. Results of version 2.1 are identical to those of version V1.0

(9) (8 corrected to 9, N.S 4/29/99) Gas transport: run the same gas transport test as the one described on p. 57-61 (use RUN 5 on p.60). Compare the results of version 2.1 with the results of version

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N.S. 4/29/99
2.03 shown on p. 61. ~~and~~ Results are identical
Results of version 2.03 on p. 61 are shown to
match an analytical solution very well,
so there N.S. 4/29/99 is no need to repeat here the
comparission with the analytical solution.

N.S 5/20/99 (10 (9)) Thermal-hydrological: run the test problems used to compare TOUGHREACT V1.0 against TOUGH2, and compare results between V.1.0 and treactq 2.1. Three problems were run: heat pipe flow to a geothermal well, and two-phase flow.
Flow to geothermal well: results of V.10 and 2.1 were identical
Heat pipe: results of V1.0 and 2.1 were identical. The run finished fine but displays an underflow error message. The same happens N.S. 4/29/99 with version 1.0. Does not happen when run ~~4~~ on my PC; does not affect results.
Two-Phase flow: results of V.10 and 2.1 were identical for the two cases in this problem (with outer ring and without outer ring). The runs finished fine but displayed the same error message as noted above for the heat pipe run, which also happens with V.1.0 and does not affect results.

N.S 5/20/99 (11 (10)) sequential iterations between ~~flow~~ transport N.S. 4/29/99 and chemistry: run the quartz dissolution problem (#2 above, on p. 68) with and without sequential iterations, and compare with analytical solution given in Johnson et al. 1998 (same as the one used for qualification of TOUGHREACT V1.0).

Problem! The outlet concentration of silica is to high when sequential iterations are used. Converges fine, but seems to dissolve too much. Needs verification and fixing.

con't 5/5/99 Fixed the problem. Notes below are for info and document further changes to the code to fix the problem. Basically, made changes to the general iterative procedure previously described in NS-1 p 138.

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To: Greg Carlisle/YM/RWDOE@CRWMS
cc: Bo Bodvarsson/YM/RWDOE@CRWMS, Mark Cushey/YM/RWDOE@CRWMS, Nancy Aden-Gleason/YM/RWDOE@CRWMS, Steve Harris/YD/RWDOE@CRWMS
From: Don Mangold/YM/RWDOE
Date: 01/24/2000 03:58:45 AM
Subject: TOUGHREACT V2.2 under Section 5.12

Greg,

Per Section 5.12 of AP-SI.1Q, below are attached the files for TOUGHREACT V2.2 to be placed under CM as unqualified software used for AMRs. It includes the SAP that describes the use and future verification of the unqualified software, a software user request, and the executable (approximately 843 KB).

If you have any questions, please fell free to contact me.

Don


SAP 5.12 trtv22.do


sur1-00 trtv22.doc


treactq2.2