QA: QA

VALIDATION TEST PLAN (VTP)
for
TOUGHREACT Version 2.2

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PRELIMINARY DRAFT
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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 Plan (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 for TOUGHREACT V2.2. In accordance with AP-SI.1Q, Rev. 2, ICN 4, *Software Management*, The VTP is preceded by Installation Test Plan (ITP) 10154-ITP-2.2-01, and represents the final document to be submitted (along with the SAP, RD, DD, and ITP) for Information Technology Software Management Analyst (ITSMA) review for Control Point 1.

1. OVERVIEW OF REQUIREMENTS

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 are to be made (see Requirements Document 10154-RD-2.2-01) 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 output file for gases, option to output gas and mineral amounts in volume fraction, output additional variables such as porosity and permeability in plot files).

For the VTP, hand-calculation is to be 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 will be used for software validation for testable requirements 1 and 8.

Test cases will be performed as described in Table 1.

1.1 Verification and Validation Plan

Table 1 lists the requirements and acceptance criteria that were established to validate TOUGHREACT V2.2. The type of requirements and acceptance criteria in Table 1 were developed to test the enhancements listed above.

2. DEVELOPED AND MODIFIED CODES

Elements of the DD for TOUGHREACT V2.2, 10154-DD-2.2-01, are addressed below.

2.1 Inputs and Outputs

The inputs and outputs requirements of the DD, Section IV, are to be tested as outputs during the course of other tests, and shall be examined by inspection.

2.2 User Interfaces

User interfaces described in the DD, Section V, are to be tested as outputs during the course of the other tests, and shall be examined by inspection

2.3 Data and Logical Model

The data and logical models described in the DD, Section VIII, are to be tested as outputs during the course of the other tests, and shall be examined by inspection.

3. TEST STEP DESCRIPTION WITH IDENTIFIER FOR EACH STEP

After installation of TOUGHREACT V2.2 (per the ITP), the following steps are to be undertaken for each verification test case:

1. Compile and execute the code.
2. Provide the appropriate test case input for that case.
3. Test the resulting output against the specified acceptance criteria.
4. Test is complete when criteria are satisfied.

4. ACCEPTANCE/REJECTION CRITERIA

4.1 Qualitative

The qualitative acceptance criterion is that the execution terminates without error.

4.2 Quantitative

For each test case, the respective acceptance criteria are listed in Table 1.

5. ACQUIRED CODE INDEPENDENT TEST CASES

Not applicable as this is a developed/modified code.

6. ACQUIRED CODE SUPPLEMENTAL TEST CASES

Not applicable as this is a developed/modified code.

7. INSTRUCTIONS FOR EXECUTION OF THE TEST CASES

All test cases must be run as specified in Section 3.0.

Reference:

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

Table 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% (this acceptance criteria is less strict than for other regression tests because this is a complex problem and the codes were set to use different solvers).	2-D vertical cross section	This report

6	Verification 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 flow 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 report
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