LABORATORY NOTEBOOK

NOTEBOOK NO. _____

CONTINUED FROM NOTEBOOK NO. _____ CONTINUED TO NOTEBOOK NO. _____

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PROJECT

This notebook documents modeling activities performed using TOUGHREACT version 3.0, a reactive transport modeling code. Most of this work is expected to be conducted under the Quantity & Chemistry integrated sub-issue (ISI) Project no. 20.06002.01.212. Modeling conducted for other projects / ISI's will be noted as part of the initial entry for that activity 3/3/06

Users

Printed name	Signature	Initials
JAMES MYERS	James L Myers	JLM

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3/3/06

TOUGHREACT version 3.0 Model Validation

The objective of this task is to run the sample problems provided as part of the TOUGHREACT program disk on an IBM-compatable PC and compare the results with the outputs provided by the code developers.

This software is not under configuration control These activities are intended to meet the documentation requires for installation and validation testing stipulated in TOP-018. It is expected that following these activities, TOUGHREACT ver 3.0 will be placed under configuration control.

The sample problems will be run on an IBM-compatible PC w/ a Windows XP operating system. In order to run the problems, the programs must be installed on the ~~d~~ JLM 3/3/06 hard drive of the user's PC. In this case the programs and sample problems are installed on the D:\ drive. TOUGHREACT is run in batch mode in the DOS operating environment Therefore, an understanding of basic DOS commands is required to use the program

This task will consist of 2 major items. The first item is ~~the~~ JLM 3/3/06 to run each of the 8 sample problems. The second is to compare the user-generated outputs w/ those provided

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Sample Problem Runs 3/7/06

The objective of this item is to use the inputs, databases, and executable files to run the eight (8) sample problems provided as part of the TOUGHREACT programs disk

An IBM-compatible PC equipped w/ a Pentium 4 processor and running Windows XP Professional operating system will be used for this activity

Procedure
The following general procedure will be used.

1. Create a folder/subdirectory for the validation test run. (eg, D:\TOUGHREACT\validation_test)

2. Create a working directory for the example problems (eg, D:\TOUGHREACT\validation_test\example_1)

3 Copy the input files and database file from the appropriate sample problem folder to the appropriate working directory

4. Copy the appropriate executable file from the \TOUGHREACT\EXE-files-PC\ folder to the working folder.

5. Open a command prompt window
the command prompt

6. Change to the working directory if necessary.

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3/7/06 Procedure (continued)

7. Run the sample problem by typing the executable file name and hitting the enter key

8. Run has completed when the command prompt appears

9. Repeat steps 2 through 8 until all eight (8) sample problems are complete.

Actual

Created directory D:\TOUGHREACT\validation_test\
(note: all examples folders are in the above folder)
Example problem P1_EOS9_kd-decay
(8.1 Aqueous Transport w/ Adsorption (linear kd) + Decay (EOS9) in users manual)
(VTP) 9LM 3/7/06
(Test case 6.2 in validation test plan for TOUGHREACT
draft 9LM 3/7/06

Create folder \example_P1\

Copy input files flow.inp, solute.inp, chemical.inp and database thermXu4.dat to \example_P1

Copy treact_eos9 to \example_P1

Run treact_eos9

treact_eos9 completed successfully.

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Actual (continued) 3/7/06

Example Problem P2_EOS9_Aqui-aquifer
(8.2 .... in users manual)
(6.3 .... in VVTP for TOUGHREACT)
draft JFM
3/7/06

Create folder \example_P2

Copy files: flow.inp, solute.inp, chemical.inp,
therm Xu4.dat, and treact_eos9 to
\example_P2

Run treact_eos9

treact_eos9 completed successfully

Example Problem P3_EOS3_YM-calcite JFM 3/7/06
JFM 3/7/06 8.3 ~~(8.2~~ ... in users manual + 6.4 ... in draft VVTP for TOUGHREACT)
Create folder - \example_P3
Copy - flow.inp, solute.inp, chemical.inp, therm208.dat
and treact_eos3 to \example_P3

Run treact_eos3

treact_eos3 completed successfully

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3/7/06 Actual (continued)

Example Problem P4_ECO4_heat-test
(8.4 in users manual + 6.5 in draft VTP for TOUGHREACT)

Created folder - \example_P4

Copied files - flow.inp, solute.inp, chemical.inp, GENER, INCON, MESH, thermk1.01.dat, and treact_eo4 to \example_P4

ran treact_eo4

treact_eo4 completed successfully

Example Problem P5_ECO2_1D-radial
(8.5 in users manual + 6.6 in draft VTP for TOUGHREACT)

Created folder \example_P5

Copied files flow.inp, solute.inp, chemical.inp, CO2TAB, thermX44.dat, + treact_ECO2 to example_P5

note: CO2TAB is a property file for CO_2 used by the ECO2 module

ran treact_eco2

treact_eco2 completed successfully

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Actual (continued) 3/7/06

Example Problem P6_EOS9_copper
(8.6 in users manual + 6.7 in VTP for TOUGHREACT)

created folder \example_P6

copied files flow.inp, solute.inp, chemical.inp
thermXu4.dat + treact_eos9 to
\example-P6

ran treact_eos9

treact_eos9 completed successfully

Example Problem P7_EOS2_LVC
(8.7 in users manual + 6.8 in draft VTP for TOUGHREACT)

created folder \example_P7

copied files flow.inp, solute.inp, chemical.inp,
thermXu4.dat + treact_eos2 to folder
\example_P7

ran treact_eos2

treact_eos2 completed successfully

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3/7/06 actual (continued)

Example Problem P8_EOS1_oxalic
(8.8 in users manual + 6.9 in draft VTP for TOUGHREACT)

created folder \example_P8

copied files flow.inp, solute.inp, chemical.inp
thermok.dat + treact_eos1

ran treact_eos1

treact_eos1 completed successfully

Comparison of Validation Test Output Files
w/ Outputs supplied w/ program

The objective of this activity is to compare the output files to determine if there is any significant difference between the validation test runs and results from the code developer

The comparison was performed using TextPad v4.7.3.
This text editor has a built-in "compare files" function

Procedure
Open files to be compared in TextPad
Select "Compare Files" from "Tools" menu
Results appear in the program window

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Output File Comparison (continued) 3/7/06

Results
The results of the file comparisons are presented below

VALIDATION TEST PROBLEM 6.2

Flow.out comparison results:

```
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 results:

```
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

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3/7/06 Output file comparison - Results (continued)

VALIDATION TEST PROBLEM 6.2 (CONTINUED)

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 results:

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 Comparison:

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

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Output file comparison - Results (cont.) 3/7/06

VALIDATION TEST PROBLEM 6.3

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

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3/7/06 Output file comparison - Results (cont.)

VALIDATION TEST PROBLEM 6.3 (continued)

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

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Output file comparison - Results (cont.) 3/7/06

VALIDATION TEST PROBLEM 6.4

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

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3/7/06 Output file comparison - Results (cont.)

VALIDATION TEST PROBLEM 6.4 (continued)

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
```

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Output file comparison - Results (cont.) 3/7/06

VALIDATION TEST PROBLEM 6.4 (continued)

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

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3/7/06 Output file comparison - Results (cont.)

VALIDATION TEST PROBLEM 6.5

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

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Output-file comparison - Results (cont.) 3/7/06

VALIDATION TEST PROBLEM 6.5 (continued)

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

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3/7/06 Output file comparison - Results (cont.)

VALIDATION TEST PROBLEM 6.6

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

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Output file comparison - Results (cont.) 3/7/06

VALIDATION TEST PROBLEM 6.6 (continued)

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

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3/7/06 Output file comparison - Results (cont.)

VALIDATION TEST PROBLEM 6.7

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

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Output file comparison - Results (cont) 3/7/06

VALIDATION TEST PROBLEM 6.7 (continued)

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

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3/8/06 Output file comparison - Results (cont.)

VALIDATION TEST PROBLEM 6.8

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

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Output file comparison - Results (cont.) 3/8/06

VALIDATION TEST PROBLEM 6.8 (continued)

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

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3/8/06 Output file comparison - Results (cont.)

VALIDATION TEST PROBLEM 6.9

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

AFM 3/8/06

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Output file comparison - Results (cont.) 3/8/06

VALIDATION TEST PROBLEM 6.9 (continued)

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

AEM 3/8/06

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BOOK NO.

PROJECT

3/31/06 Drift-Scale Thermal Hydrological Chemical (THC) Modeling

The purpose of this activity is to conduct coupled reactive transport modeling using TOUGHREACT and the modeling assumptions and approximations described in the DOE's Drift-Scale THC seepage model report (MDL-NBS-HS-000001 REV4) The results of this modeling will be compared to those presented in the above report to evaluate the DOE's model + modeling process

TOUGHREACT version 3.0 is not currently under configuration control. The software validation report is currently in review and the software ~~will~~ QRM 4/3/06 is expected to be under configuration control and fully validated in the near future. The modeling will be performed on an IBM-compatable PC ~~running~~ QRM 4/3/06 running Windows XP operating system.

The flow mesh that will be used was developed by Alex Sun and is based a previously developed flow mesh for Multiflo by Randy Fedors. The documentation for the Multiflo mesh can be found in scientific notebook 432E vol VII ~~as~~ QRM 4/3/06 A description of the current flow mesh will be provided below

Various other model input QRM 4/3/06 parameters will be provided below.

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THC Modeling (cont.)

4/4/06

As a starting point for this modeling activity I will use three input files provided by Alex Sun. These files are: D:\THC Modeling\ flow.inp, solute.inp, + chemical.inp. A description of the input parameters is detailed below

4)

flow.inp

ROCKS (material parameters for reservoir domains)

This section contains 79 model domains. About half are matrix domains + half are fracture. It appears that this flow.inp file was built from the flow.inp file ~~provided~~ GLM 4/4/06 for sample problem 3 provided w/ the program. Only ~~45~~ GLM 4/4/06 31 of domains are called up in mesh defined in the ELEME section of this input file. This flow mesh uses the evelations presented in figure 6.5-1 (MDL-NBS-HS-00001 REV4). A summary of this data along w/ the CNWRA model mesh info is presented in the table on p. 28.

It is not clear why several of the DOE model layers/rock types have been omitted from this input file. This will require further review.

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PROJECT

THC Modeling (cont.)

4/4/06

DOE's* Model Layer	Top of Layer* Elevation (m)	Mesh Top of Layer* Z Coordinate (m)	CNWRA Model Layer	starting node	ending node	total nodes
Top	1446.6	363.8				
tcw11	1446.6	363.8	tcw1	857	892	36
tcw12	1419.2	336.4	tcw2			
tcw13	1342.1	259.3	tcw3	845	856	12
ptn21	1326.5	243.7	ptn1	833	844	12
ptn22	1323.1	240.3	ptn2			
ptn23	1321	238.2	ptn3			
ptn24	1318.2	235.4	ptn4			
ptn25	1312.7	229.9	ptn5			
ptn26	1303.6	220.8	ptn6			
tsw31	1294.1	211.3	tsw1	821	832	12
tsw32	1279.7	196.9	tsw2	809	820	12
tsw33	1249.3	166.5	tsw3	761	808	48
tsw34	1169.2	86.4	tsw4	725	760	36
tsw35	1132	49.2	tsw5	689	724	36
Drift center	1082.8	0		1	556	556
tsw36	1030.6	-52.2	tsw6	557	592	36
tsw37	997.4	-85.4	tsw7			
tsw38	980.8	-102	tsw8	593	604	12
tsw39	967	-115.8	tsw9			
ch1v	956.9	-125.9	ch1	605	616	12
ch2v	945.2	-137.6	ch2	617	640	24
ch3v	931.9	-150.9	ch3			
ch4z	919.2	-163.6	ch4			
ch5z	906.4	-176.4	ch5			
ch6	892.4	-190.4	ch6	641	652	12
pp4	878.5	-204.3	pp4			
pp3	865.9	-216.9	pp3			
pp2	833.2	-249.5	pp2			
pp1	818.2	-264.6	pp1	653	688	36
bf3	756.7	-326.1				
Bottom	730	-352.8				

* data from Figure 6.5-1 of DOE report #MDL-NBS-HS-000001 REV4

Given the uncertainties about this flow mesh and the fact that Alex Liu is not available to work on this activity, I am going to discuss the objectives w/ Scott Painter to determine if there is a better approach.

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4/4/06 WZB

[redacted]

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BOOK NO. PROJECT

Reactive Transport Modeling of Integrated Tests 4/17/06

As part of the proactive work in the FY06 CPS plan center staff is conducting a series of experiments that simulate unsaturated flow through porous media, into and around a simulated drift opening, and interaction with a heated simulated waste package and/or drip shield. As part of the initial work plan center staff are performing flow modeling in order to properly design the experimental set up.

The purpose of this activity is to conducted reactive transport modeling of the experimental system in order to predict chemical interactions between the infiltrating water and the porous media. Currently, the work plan calls for three water compositions (see below) and two porous medias (quartz + crushed tuff from YUCCA Mtn). The heated simulated WP/DS will create nonisothermal conditions in the experimental system

It is expected, based on similar experimental + modeling studies, that the infiltrating water will ~~react~~ JLM 4/17/06 equilibrate with the porous media. Dissolved quartz in the water will precipitate in the dryout zone (T > 100°C) surrounding the simulated heated drift.

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BOOK NO.

PROJECT

4/17/06 Modeling of Integrated Tests (cont.)

TOUGHREACT Ver 3.0 will be used for this modeling activity. TOUGHREACT is not currently under configuration ~~controlled~~ JEM 4/17/06 control. The validation report is currently in review, and is expected to be final in the near future. A similar modeling exercise will be conducted using the Multiflo reactive transport code and the results of the two codes will be compared.

The flow mesh used in this activity will be developed by Chandrika Manepalley. The solute (transport) and chemistry input files/parameters will be discussed below. A brief description of the flow input will be recorded along with a reference to the appropiate scientific notebook containing a complete description.

Chemistry (Chemical inp)

The chemistry of the infiltrating water and the ~~chem~~ JEM 4/17/06 mineralogy of the porous media is contained in the chemical.inp file in TOUGHREACT. Three (3) water chemistries will be considered as part of this modeling activities. The compositions span the range of expected pH at the YUCCA mtn and were selected by Bobby Pabalan.

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BOOK NO. PROJECT

Modeling Integrated Tests (cont.) 4/17/06
Infiltration Water Chemistries

StreamAnalyzer charge balanced output

SD-6/443.5 (neutral type)

pH calc	7.79	
Na+1	2.980E-03	molarity
K+1	1.023E-04	molarity
Mg+2	4.814E-04	molarity
Ca+2	1.203E-03	molarity
Cl-1	1.334E-03	molarity
SO4-2	1.020E-03	molarity
NO3-1	1.387E-03	molarity
HCO3-1	1.655E-03	molarity
CO3-2	1.666E-05	molarity

NRG-6/158.2 (Ca-Cl type)

pH calc	7.89	
Na+1	1.549E-03	molarity
K+1	0.000E+00	molarity
Mg+2	9.587E-04	molarity
Ca+2	3.068E-03	molarity
Cl-1	5.218E-03	molarity
SO4-2	1.655E-03	molarity
NO3-1	5.161E-04	molarity
HCO3-1	5.572E-04	molarity
CO3-2	0.000E+00	molarity

UZ#16/1343.7 (alkaline type)

pH calc	10.02	
Na+1	4.306E-03	molarity
K+1	0.000E+00	molarity
Mg+2	9.875E-05	molarity
Ca+2	4.242E-04	molarity
Cl-1	1.580E-03	molarity
SO4-2	2.394E-04	molarity
NO3-1	2.903E-04	molarity
HCO3-1	7.801E-04	molarity
CO3-2	1.112E-03	molarity

Excel-derived recipes

SD-6/443.5 (neutral)	**molarity**
pH calc	7.78
MgSO4	4.8138E-04
K2SO4	5.1153E-05
Na2SO4	4.8763E-04
CaCl2	6.6708E-04
Ca(NO3)2	5.3557E-04
NaNO3	3.1585E-04
NaHCO3	1.6886E-03

NRG-6/158.2 (Ca-Cl)	**molarity**
pH calc	7.89
CaCl2	2.6091E-03
Ca(NO3)2	2.5804E-04
CaSO4	2.0086E-04
NaHCO3	5.5722E-04
Na2SO4	4.9564E-04
MgSO4	9.5865E-04

UZ#16/1343.7 (alkaline)	**molarity**
pH calc	10.49
CaCl2	4.2417E-04
MgCl2	9.8745E-05
NaCl	5.3372E-04
NaNO3	2.9030E-04
Na2SO4	2.3943E-04
Na2CO3	3.0034E-03

4/17/06 J.L. Myers

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4/17/06 Modeling of Integrated Tests (cont.)

Chemical.inp (cont.)

Copied the chemical.inp from sample problem P4_EOS4_Leat test to D:\Integrated Testing\TOUGHREACT Modeling\Quartz\neutral_qtz\ and implement the following changes:

- deleted alO2-, f-, hfeO2(aq) from 'Primary aqueous species'

- deleted hematite, hydglassfe3 from 'Minerals"

- changed "ctot" ~~aqueous~~ aqueous concentrations to the values in the table on p. 31 QZM 4/17/06
  - note: the values ~~on~~ p. 31 are molarity (mol/l). These concentrations were converted to molality (mol/1000g) by assuming T=25°C and the density of H_2O (solvent) is 1000g/l. This approximation is assumed to decrease the actual concentrations about 0.3%

  - The conc. of SiO2(aq) was not changed, because an initial value was not provided in the table on p. 31. An ~~on~~ QZM 4/17/06 initial value will be selected after further discussions w/ Bobby Pabalan.

All 'Initial mineral zones' deleted, except 'quartz'
- mol fraction changed to 1.00000
- the surface area of quartz was left at 300 cm^2/g mineral
  - this value may be changed based on actual properties of porous media used in experiments.

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Modeling of Integrated Tests (cont.) 4/17/06

Chemical.inp (cont.)

- "Initial gas zones"
  - $CO_2(g)$ changed to partial pressure = $3.163e^{-4}$

- all other values unchanged at this time

- 'Permeability - Porosity Zones'
  - 13 zones deleted of 14 initially present
  - 1 zone remains

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5/16/06

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PROJECT

5/16/06 Modeling of Integrated Tests (cont.)

Flow (flow.inp)

The flow mesh and hydrologic properties are contained in the flow.inp file in TOUGHREACT. The flow mesh is based on work by Chandrika Manepaly for MULTIFLO, and is documented in scientific notebook . Details are provided here also. The steps used to generate this input file are provided below

Copied a flow.inp file from D:\TOUGHREACT_Course\day-1\section-4_Plug flow\quartz\ to D:\Integrated Testing\TOUGHREACT Modeling\. This input file was originally generated for a fully saturated flow through a column packed w/ crushed quartz.

5/17/06 Cut the "ELEME" and "CONNE" data blocks and pasted them at bottom of the file below the "ENDCY" command. ~~The data will not be read~~ RM 5/16/06 Any data below the "ENDCY" command will not be read as part of the input to TOUGHREACT.

Changed ENDCY to ENDFI - this tells TOUGHREACT to stop after mesh generation, without executing flow.

Ran TOUGHREACT using treact_eos3 command in DOS window

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Run completed successfully, generating MESH file. 5/17/06

Prior to running program I inserted the following

```
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
          0.
NX       12        0.05
NY        1        0.05
NZ       24        0.05
```

JLM 5/17/06

The above section creates a grid that is 12 x 24 cells in X-direction (horizontal) and Z-direction (vertical), respectively. The cell size is 0.05 m (50 cm) in the X, Y, & Z directions. This is a structured or cartesian mesh.

TOUGHREACT generated the mesh shown below. Flow is permitted between cells that share a common side.

The cells were manually renamed from the default names to Chandrika's numbering for easy comparison of results between equivalent TOUGHREACT & MULTIFLO simulations.

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5/17/06 Modeling Integrated Tests (cont.)

TOUGHREACT mesh grid naming

X-direction →

A11 1	A11 2	A11 3	A11 4	A11 5	A11 6	A11 7	A11 8	A11 9	A1110	A1111	A1112
A21 1	A21 2	A21 3	A21 4	A21 5	A21 6	A21 7	A21 8	A21 9	A2110	A2111	A2112
A31 1	A31 2	A31 3	A31 4	A31 5	A31 6	A31 7	A31 8	A31 9	A3110	A3111	A3112
A41 1	A41 2	A41 3	A41 4	A41 5	A41 6	A41 7	A41 8	A41 9	A4110	A4111	A4112
A51 1	A51 2	A51 3	A51 4	A51 5	A51 6	A51 7	A51 8	A51 9	A5110	A5111	A5112
A61 1	A61 2	A61 3	A61 4	A61 5	A61 6	A61 7	A61 8	A61 9	A6110	A6111	A6112
A71 1	A71 2	A71 3	A71 4	A71 5	A71 6	A71 7	A71 8	A71 9	A7110	A7111	A7112
A81 1	A81 2	A81 3	A81 4	A81 5	A81 6	A81 7	A81 8	A81 9	A8110	A8111	A8112
A91 1	A91 2	A91 3	A91 4	A91 5	A91 6	A91 7	A91 8	A91 9	A9110	A9111	A9112
AA1 1	AA1 2	AA1 3	AA1 4	AA1 5	AA1 6	AA1 7	AA1 8	AA1 9	AA110	AA111	AA112
AB1 1	AB1 2	AB1 3	AB1 4	AB1 5	AB1 6	AB1 7	AB1 8	AB1 9	AB110	AB111	AB112
AC1 1	AC1 2	AC1 3	AC1 4	AC1 5	AC1 6	AC1 7	AC1 8	AC1 9	AC110	AC111	AC112
AD1 1	AD1 2	AD1 3	AD1 4	AD1 5	AD1 6	AD1 7	AD1 8	AD1 9	AD110	AD111	AD112
AE1 1	AE1 2	AE1 3	AE1 4	AE1 5	AE1 6	AE1 7	AE1 8	AE1 9	AE110	AE111	AE112
AF1 1	AF1 2	AF1 3	AF1 4	AF1 5	AF1 6	AF1 7	AF1 8	AF1 9	AF110	AF111	AF112
AG1 1	AG1 2	AG1 3	AG1 4	AG1 5	AG1 6	AG1 7	AG1 8	AG1 9	AG110	AG111	AG112
AH1 1	AH1 2	AH1 3	AH1 4	AH1 5	AH1 6	AH1 7	AH1 8	AH1 9	AH110	AH111	AH112
AI1 1	AI1 2	AI1 3	AI1 4	AI1 5	AI1 6	AI1 7	AI1 8	AI1 9	AI110	AI111	AI112
AJ1 1	AJ1 2	AJ1 3	AJ1 4	AJ1 5	AJ1 6	AJ1 7	AJ1 8	AJ1 9	AJ110	AJ111	AJ112
AK1 1	AK1 2	AK1 3	AK1 4	AK1 5	AK1 6	AK1 7	AK1 8	AK1 9	AK110	AK111	AK112
AL1 1	AL1 2	AL1 3	AL1 4	AL1 5	AL1 6	AL1 7	AL1 8	AL1 9	AL110	AL111	AL112
AM1 1	AM1 2	AM1 3	AM1 4	AM1 5	AM1 6	AM1 7	AM1 8	AM1 9	AM110	AM111	AM112
AN1 1	AN1 2	AN1 3	AN1 4	AN1 5	AN1 6	AN1 7	AN1 8	AN1 9	AN110	AN111	AN112
AO1 1	AO1 2	AO1 3	AO1 4	AO1 5	AO1 6	AO1 7	AO1 8	AO1 9	AO110	AO111	AO112

Z-direction ↓

Chandrika's mesh grid naming

X-direction →

00001	00002	00003	00004	00005	00006	00007	00008	00009	00010	00011	00012
00013	00014	00015	00016	00017	00018	00019	00020	00021	00022	00023	00024
00025	00026	00027	00028	00029	00030	00031	00032	00033	00034	00035	00036
00037	00038	00039	00040	00041	00042	00043	00044	00045	00046	00047	00048
00049	00050	00051	00052	00053	00054	00055	00056	00057	00058	00059	00060
00061	00062	00063	00064	00065	00066	00067	00068	00069	00070	00071	00072
00073	00074	00075	00076	00077	00078	00079	00080	00081	00082	00083	00084
00085	00086	00087	00088	00089	00090	00091	00092	00093	00094	00095	00096
00097	00098	00099	00100	00101	00102	00103	00104	00105	00106	00107	00108
00109	00110	00111	00112	00113	00114	00115	00116	00117	00118	00119	00120
00121	00122	00123	00124	00125	00126	00127	00128	00129	00130	00131	00132
00133	00134	00135	00136	00137	00138	00139	00140	00141	00142	00143	00144
00145	00146	00147	00148	00149	00150	00151	00152	00153	00154	00155	00156
00157	00158	00159	00160	00161	00162	00163	00164	00165	00166	00167	00168
00169	00170	00171	00172	00173	00174	00175	00176	00177	00178	00179	00180
00181	00182	00183	00184	00185	00186	00187	00188	00189	00190	00191	00192
00193	00194	00195	00196	00197	00198	00199	00200	00201	00202	00203	00204
00205	00206	00207	00208	00209	00210	00211	00212	00213	00214	00215	00216
00217	00218	00219	00220	00221	00222	00223	00224	00225	00226	00227	00228
00229	00230	00231	00232	00233	00234	00235	00236	00237	00238	00239	00240
00241	00242	00243	00244	00245	00246	00247	00248	00249	00250	00251	00252
00253	00254	00255	00256	00257	00258	00259	00260	00261	00262	00263	00264
00265	00266	00267	00268	00269	00270	00271	00272	00273	00274	00275	00276
00277	00278	00279	00280	00281	00282	00283	00284	00285	00286	00287	00288

Z-direction ↓

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Modeling Integrated Tests 5/18/06
Flow.inp (cont.)

Modified the Flow.inp file w/ the following values. Most values from Chandrika Manepaly and are documented in Input Details.xls.

ROCKS (material ~~parameters~~ GRM 5/18/06 parameters for reservoir domains)

Rock type (MAT) : rock1
5/18/06 NAD : 1 = read another record to override defaults
(DROK) Rock ~~gar~~ GRM grain density : 2000 kg/m^3
default porosity (POR) : 0.43

Permeability (PER(I), I=1,3) = 1.00×10^{-11} m^2

heat conductivity (CWET) = 2.7 W/m °C
(fully liq. saturation)

rock grain specific heat (SPHT) 840 J/kg °C

All other values in the ROCKS category were set to default values.

PARAM (computation parameters, time stepping info., and default initial conditions)

KDATA (amt of printout) = ~~4~~ 3 Changed value based on email response from Tianfu Xu (see p 40 for response.) GRM 5/22/06

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5/19/06 Modeling Integrated Tests
Flow.inp
PARAM (cont.)

MCYC (max. number time steps) = 9999 This tells TOUGHREACT that max. simulation time is controlled by TIMAX.

TEXP = 2.334 parameter for T dependance of gas phase diffusion coefficient. This value has no effect because diffusion is turned off (see below).

TSTART = 0.0 starting time of simulation in seconds

TIMAX = 3.6×10^3 time (sec.) simulation should stop

DELTEN = 1 length of time steps (seconds)

DELTMX = 5 upper limit of time step size (sec)

GF = -9.806650 magnitude of gravity vector (m/sec^2)

All other values left as defaults.

REACT (Reactive transport simulation parameters)

MOPR(1) = 0 perform reactive transport

MOPR(2) = 0 transport data will not be written to runlog.out file (For debugging uses only)

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Modeling Integrated Tests 5/19/06
Flow.inp
REACT (cont.)

MOPR(3) = 0 source terms and other data will not be ~~a~~ QRM 5/19/06 written to runlog.out (For debugging uses only.)

MOPR(4) = 0 forces at least 1 fluid flow step to be calculated

MOPR(5) = 0 rel. ~~permeability~~ QRM permeability and capillary pressure subroutines from TOUGH2 are used

MOPR(6) = 0 no Leverett scaling for capillary P when porosity + permeability change as a result of mineral precipitation or dissolution

MOPR(7) = 0 specifies that 4 digits past decimal pt will be printed in chemical output files.

MOPR(8) = 0 no output files will be created containing mass balance and mineral saturation index vs. grid block at specified times.

TIMES (allows user to obtain printout at specified times)

ITI = 15 number of times (total) printout is ~~desired~~ prescribed QRM 5/22/06
QRM 5/22/06 ~~Actual~~ Actual times specified below.

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5/22/06 Modeling Integrated Tests (cont.)

Jim Myers

From: Tianfu Xu [Tianfu_Xu@lbl.gov]
Sent: Friday, May 19, 2006 4:46 PM
To: jmyers@cnwra.swri.edu
Subject: Re: TOUGHREACT KDATA = 4?

Jim,

I just got 4 runs for the sample problem 1 with KDATA = 1, 2, 3, or 4. I found level of output KDATA = 4 is the same as that of KDATA = 3. I did this sample problem some 6 years ago. I cannot remember why I used KDATA = 4. Usually I use KDATA = 2. I suggest you specifiy value of KDATA acccording to TOUGH2 V2 manual. I'll correct this for future course and sample problems.

Thanks !
-- Tianfu.

Tianfu Xu, Ph.D
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Berkeley, California 94720

Tel: +1-510-4867057
Fax: +1-510-4865686
Email: Tianfu_Xu@lbl.gov
<!--[if !supportLineBreakNewLine]-->
<!--[endif]-->

Information on TOUGHREACT is available

<> on http://www-esd.lbl.gov/TOUGHREACT/

5/22/06 JZM

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Modeling Integrated Tests 5/22/06
Flow.inp
TIMES (cont.)

iTE = blank (default) total number of times desired. ($|IT| \leq ITE \leq 100$; default is $ITE = |IT|$)

DELAF = blank (default) max time step size after any of the prescribed times have been reached (default = infinite)

TINTER = blank (default) time increments for times w/ index $|IT|, |IT|+1, \ldots, ITE$

TIS(1,15) = 0.01, 0.1, 0.5, 0.75, 1.0, 10.0, 20.0, 30.0, 40.0, 50.0, 60.0, 70.0, 80.0, 90.0, 100.0.
list of times (in ascending order) at which printout is desired.

MULTI (permits user to specify the no. + nature of balance equations that will be solved

NK = 2 (default) no. of mass components

NEQ = 3 (default) no of bal. eq / grid block. Usually NEQ = NK+1, for solving NK mass and 1 energy balance eq. Some EOS modules allow NEQ=NK, no E bal. eq. solved (isothermal problems)

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Integrated Testing
MULTI (cont.)

NPH = 2 (default) no. of phases that can be present

NB = 6 (default) no of secondary parameters in PAR-array other than component mass fractions.
Available options NB=6 (no diffusion) + NB=8 (include diffusion)

GENER (introduces sinks or sources)

EL, NE = 00001 code name of element containing sink/source. This is the source term for water infiltrating into the flow mesh from the top.

SL, NS = INF01 code name of sink/source

NSEQ = 11 number of additional sinks/sources w/ the same injection rate

NADD = 1 increment between the code numbers of ~~elements~~ two successive elements w/ identical sink/source
QRM 5/25/06

LTAB = 1 number of points in table of generation rate vs time.

TYPE = WATE specifies diff options for fluid or heat production + injection.

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Modeling Integrated Tests 5/25/06
GENER (cont.)

$GX = 9.65 \times 10^{-7}$ const. generation rate; pos. for injection, neg. for production. units kg/sec. This rate is based on a total infiltration rate of 1 l/day. This is converted by multiplying by the density of water ≅ 1 kg/l

$1\ l/day \times 1\ kg/l \div 86400\ sec/day = 1.16 \times 10^{-7}\ kg/sec$

The total generation rate must be distributed across the top of the flow grid (12 cells) ~~by~~ GLM 5/25/06

$1.16 \times 10^{-7}\ kg/sec \div 12\ cells = \boxed{9.65 \times 10^{-7}\ kg/sec/cell}$

$EX = 0.7561 \times 10^5$ fixed specific enthalpy [J/kg] of the fluid for mass injection (GX > 0). Based on the specific enthalpy for water at 80°C EX = 3.3496×10^5 J/kg (www.thermexcel.com/english/tables/eau_atm.htm) GLM 5/25/06 this EX value of 0.7561×10^5 is actually cal/kg. This isn't important for an isothermal simulation, but is a half order of magnitude too low for a non-isothermal run.

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Modeling Integrated Testing
Flow.inp (cont.)

Deleted MESHMaker section from file.
- TOUGHREACT will read the previously generated and modified MESH file

Changed "ENDFI" to "ENDCY"
- This tells ~~tough~~ GEM 5/26/06 TOUGHREACT to run a full simulation, not to stop after generating a flow mesh.

SOLUTE.INP (Transport Input)

Options for reactive geochemical transport

ISPIA = 2 flag for iteration between transport and reaction. 2 = sequential no iteration (normal value).

INIBOUND = 1 indicator of identifying boundary water solution. 1 = identifying (normally used)

ISOLVC = 5 flag for linear equation solver for transport. 5 = DLUSTB, a stabilized bi-conjugate gradient solver.

RCOUR = 0.00 both variable + flag to limit time step size. Disabled if RCOUR = 0.0

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Modeling Integrated Testing 5/26/06
SOLUTE.INP (cont.)

NGAS1 = 0 inclusion of gaseous chemical species transport. 0 = not included

ICHDUMP = 0 flag to enable printout of chemical speciation results. 0 = disabled

KCPL = 0 flag to consider feedback effects of changes that result from mineral precipitation + dissolution. 0 = disabled

ICO2H2O = 0 flag to consider effects of ~~co~~ 4LM 5/26/06 CO_2 + H_2O rxn sink/source terms on fluid flow calcs. 0 = effects ignored

NUMDR = 0 flag for calculation of derivatives of mineral kinetic rates w/ respect to conc of primary species. 0 = analytical method (normally used)

Constraints for chemical solver

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~~SL1MIN = 1x10^-4~~

The following three (3) parameters are used to skip geochemical speciation where conditions are outside the valid range for the model.

SL1MIN = 1×10^{-4} geochem. calcs are skipped when liq. sat is less than SL1MIN.

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Solute.inp (cont.)

D1MIN = 0.0 (disabled) geochem calcs are skipped when the min dist to the center of any adj grid block is less than D1MIN

STIMAX = 2.0 geochem calcs are skipped when the ionic strength is more than STIMAX. STIMAX can be up to 6 m for NaCl-dominant solns. STIMAX should not be > 2.0 m for other solns.

Read input and output file names
This section contains the user specified names for the thermodynamic database and various output files. The ~~on~~ 4LM 5/26/06 description of each file is ~~f~~ 4LM 5/26/06 provide as a comment following the file name. (see below)

Weighting Parameters + Diffusion Coefficients

WTIME = 1.0 time weighting factor
WTIME = 1.0 is suggested

WUPC = 1.0 upstream weighting factor
WUPC = 1.0 (fully upstream) is suggested

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Modeling Integrated Testing 5/26/06
Solute.inp (cont.)

DIFUN = 1×10^{-9} [m^2/s] diffusion coefficient for aqueous species. This value is inconsequential because diffusion is not currently considered

DIFUNG = 0 [m^2/s] diff coef. for gaseous species

Data for convergence criteria:

MAXITPTR = 1 max no. of seq iterations btwn transport + chemistry. If MAXITPTR = 1, a seq. non iterative approach is used where transport + chem. are solved seq. w/o iteration (normally suggested).

TOLTR = 1×10^{-3} rel. tolerance of aq. conc. for seq. transport/chem. convergence. a value between 1×10^{-3} + 1×10^{-6} is suggested

MAXITPCH = 300 max no. of iterations allowed for solving whole geochem sys.

TOLCH = 0.100×10^{-4} rel. tolerance of aq. conc. for whole chem sys. a value btwn 10^{-3} + 10^{-6} is suggested.

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Modeling Integrated Testing
dolute.inp (cont.)

MAXITPAD = 30 max no. of iter. allowed for solving sorption via surface complexation SCM not currently available in TOUGHREACT.

TOLAD = 0.1×10^{-5} rel. tolerance of ag conc. for sorption convergence

TOLDC = ϕ rel. conc change tolerance for quasi-stationary state (QSS) QSS not used.

TOLDR = 0 rel dissolution +/or precip rate change tolerance for QSS (not used).

Writing control variables
GRM 5/30/06

NWT1 = ~~8~~ 15 printout freq. (as no. of time steps) for selected grid blocks (NWNOD)

NWNOD = 4 number of grid blocks for time evolution printout.

NWCOM = 1 number of chemical components for printout

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NWMIN = +2 number of minerals for printout

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Modeling Integration Testing
Solute.inp (cont.)

IWCOMT = 1 printout of total aqueous component concentrations

ICONFLAG = 0 flag for aq conc. units in output files
0 ≡ mol/kg H_2O 1 ≡ mol/l liquid

MINFLAG = flag for units of mineral abundances in output files.

pointer of nodes for writing in time (Five-character name of a grid block)
00006 00066 00138 00282

pointer of components for writing (vector component numbers from chemical.inp file. The vector component number is determined from its position in the listing of 'Primary Aqueous Species' in the chemical.inp file

7 (≡ SiO_2 (aq))

pointer of minerals for writing (vector component numbers of minerals from the 'Mineral' listing in the chemical.inp file.)
12 18

s 5/30/06 default values of chemical zone codes for grid blocks (default values for the following records)

IZIWDF = 1	initial water zone number
IZBWDF = 1	boundary inflow (including injection at internal blocks) water zone no
IZMIDF = 1	mineral zone no.
IZGSDF = 1	gas zone no
IZADDF = 0	adsorption zone no
IZEXDF = 0	ion exchange zone no.
IZPPDF = 1	zone no. for porosity-perm rel.
IZKDDF = 1	linear adsorption K_d zone no.

Chemical ~~propertt~~ QLM 5/30/06 property zone related to grid blocks

- no values specified. Default values will used for all grid blocks

List of grid blocks connected to constant pressure boundary of gaseous species

- no values specified. It is assumed that all cells are in equil. w/ atmosphere.

All these input files have been ~~updat~~ QLM 5/31/06 updated at this time (flow.inp, solute inp, + chemical.inp).

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Modeling Integrated Tests 5/31/06
Input files
Each input file is presented below.

```
flow.inp                                                                    5/25/2006

Integrated Tests 04/06: Quartz; pure water initial pH=7.78(notebook:780)
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*---
-8
rock1     1      2000.       .430  1.00E-11  1.00E-11  1.00E-11  2.70E+00
840.0
   0.0        0.0        0.0            0.0

START
PARAM----1----*-123456789012345678901234----*----5----*----6----*----7----*---
-8
   39999    99990000000000000020571003000   2.14e-5      2.334        0.0
 0.00000E0 3.600E+03    1.E+00    5.E+00dummy       -9.806650
    1.E-06
              8.3E+6           0.00000       2.39E2

REACT----1MOPR(20)-2----*----3----*----4----*----5----*----6----*----7----*---
-8
00000000


TIMES
   15
      0.01        0.1        0.5       0.75        1.0       10.0       20.0
      30.0
      40.0       50.0       60.0       70.0       80.0       90.0      100.0

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*---
-8
    2    3    2    6


GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*---
-8
00001INF01   11    1          1     WATE 9.65000E-70.7561E+05    0.


ENDCY
```

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Integrated Tests Modeling
solute.inp Input File

```
solute.inp                                                                    5/30/2006

'Integrated Tests 04/06: Quartz; pure water initial pH=7.78(notebook:780)'
options for reactive chemical transport
    2    1    5 0.00    0    0    0    0    0 ! ISPIA,INIBOUND,ISOLVC,rcour,NGAS1,ichdump,kcpl,Ico2h2o,numdr
constraints for chemical solver (3e10.4)
   1.00e-4   0.000     2.0                !s11min, dlmin, stimax
Read input and output file names:
ther_ympR4a.dat                  ! thermodynamic database
iter.dat                         ! iteration information
tec_conc.dat                     ! aqueous concentrations in tecplot form
tec_min.dat                      ! mineral data  in tecplot form
tec_gas.dat                      ! gas data in tecplot form
time.dat                         ! concentrations at specific elements over time
Weighting parameters
       1.0       1.0    1.d-09       0.0    ! itime wupc,dffun,dffung
data for convergence criteria:
    1 0.100E-03  300 0.100E-04   30 0.100E-05  0.00E-05  0.00E-05
    !MAXITPR,TOLTR,MAXITPCH,TOLCH,MAXITPAD,TOLAD,TOLDC,TOLDR
writing control variables:
   15    4    1    1    1    0    1   ! NWTI,NWNOD,NWCOM,NWMIN,IWCOMT,conflag(=1:mol/l),minflag(=1:Vf)
pointer of nodes for writing in time:
00006000660013800282
pointer of components for writing (15 per line, 15I5):
    3
pointer of minerals for writing (20 per line, 20I5):
   12   18
default values of chemical zone codes for grid blocks:
    1    1    1    1    0    0    1    1
chemical zone codes for nodes:

nodes connected to gas supply (i.e.) atmosphere

end
```

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Flow.inp Input Chemical

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chemical.inp 5/30/2006

```
'Integrated Tests 04/06: Quartz; neutral water initial pH=7.78(notebook:780)'
'-----------------------------------------------------------------------------
'
'DEFINITION OF THE GEOCHEMICAL SYSTEM'
'PRIMARY AQUEOUS SPECIES'
'h2o'
'h+'
'ca+2'
'mg+2'
'na+'
'cl-'
'sio2(aq)'
'hco3-'
'so4-2'
'k+'
'no3-'
'*'
'MINERALS'
'gypsum' 0 0 0 3
0. 0. 0.
'calcite'    0 0 0 2
1.06  25. 200.
'microcline-b'   1 3 0  0
1.78e-13 0 1.0 1.0 36. 0.0 0.0 0.0
1.78e-13 0 1.0 1.0 36. 0.0 0.0 0.0  1.e-6   0
0.0   0.    000.00
'albite-low'   1 3 0  0
7.08e-13 0 1.0 1.0 67.7  0.0 0.0 0.0
7.08e-13 0 1.0 1.0 67.7  0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'anorthite'    1 1 0  0
3.16e-15 0 1.0 1.0 67.7  0.0 0.0 0.0
'smect-ca-cal'     1 3 1 0
2.00e-14 0 1.0 1.0 58.6  0.0 0.0 0.0
2.00e-14 0 1.0 1.0 58.6  0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'smect-na-cal'     1 3 1 0
2.00e-14 0 1.0 1.0 58.6  0.0 0.0 0.0
2.00e-14 0 1.0 1.0 58.6  0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'smect-mg-cal'     1 3 1 0
2.0e-14 0 1.0 1.0 58.6  0.0 0.0 0.0
2.0e-14 0 1.0 1.0 58.6  0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'illite'     1 3 0  0
2.0e-14 0 1.0 1.0 58.6  0.0 0.0 0.0
2.0e-14 0 1.0 1.0 58.6  0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'tridymite'  1 1 0  0
3.45e-13 0 1.0 1.0 68.9  0.0 0.0 0.0
'cristoba-a'  1 1 0  0
3.45e-13 0 1.0 1.0 68.9  0.0 0.0 0.0
'quartz'       1 1 0  0
```

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5/31/06 Chemical.inp (cont)


```
4.52e-14 0 1.0 1.0 90.1 0.0 0.0 0.0
'stell/10-r02'   1 3 0  0
5.66e-13 0 1.0 1.0 58.0 0.0 0.0 0.0
5.66e-13 0 1.0 1.0 58.0  0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'heul/10-r02'   1 3 0  0
5.66e-13 0 1.0 1.0 58.00 0.0 0.0 0.0
5.66e-13 0 1.0 1.0 58.00 0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'mord/10-r02'    1 3 0  0
5.66e-13 0 1.0 1.0 58.00 0.0 0.0 0.0
5.66e-13 0 1.0 1.0 58.00 0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'clpt/10-r02'   1 3 0  0
2.37e-13 0 1.0 1.0 58.00 0.0 0.0 0.0
2.37e-13 0 1.0 1.0 58.00 0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'kaolinite'    1 3 0  0
1.00e-13  0 1.0 1.0 7.1 0.0 0.0 0.0
1.00e-13  0 1.0 1.0 7.1 0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'sio2(amor.)'   1 3 0  1
7.32e-13 0 1.0 1.0 60.9 0.0 0.0 0.0
1.00e-10 0 1.0 4.4 0.0 0.0 0.0 0.0  1.e-4   1
0.0 0.0 0.0
'opal_proxy'   1 1 0  0
7.32e-13 0 1.0 1.0 60.9 0.0 0.0 0.0
'sepiolite'  1 3 0  0
2.67e-14 0 1.0 1.0 58.6  0.0 0.0 0.0
2.67e-14 0 1.0 1.0 58.6  0.0 0.0 0.0  1.e-6   0
0.0 0.0 0.0
'nano3'  1 3 0  7
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0  1.e-6   0
0. 0. 0.
'kno3'  1 3 0 6
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0  1.e-6   0
0. 0. 0.
'halite'  1 3 0 11
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0  1.e-6   0
0. 0. 0.
'sylvite'  1 3 0 12
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0  1.e-6   0
0. 0. 0.
'mgso4' 1 3 0 10
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0  1.e-6   0
0. 0. 0.
'k2so4' 1 3 0  8
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0
```

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PAGE

Chemical.inp (cont.) 5/31/06

```
chemical.inp                                                          5/30/2006

1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0  1.e-6   0
0. 0. 0.
'na2so4' 1 3 0  9
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0
1.00e-6 0 1.0 1.0 0.0 0.0 0.0 0.0  1.e-6   0
0. 0. 0.
'*'                 0   0  0 0
'GASES'
'co2(g)' 0
'*'
'SURFACE COMPLEXES'
'*'
'species with Kd and decay    decay constant(1/s)'
'*'                     0.0d0
'EXCHANGEABLE CATIONS'
'                 master     convention     ex. coef.'
'*'                 0            0            0.0
'-----------------------------------------------------------------------'
'INITIAL AND BOUNDARY WATER TYPES'
1   1     !niwtype, nbwtype, nrwtype= number of ini, bound, rech waters
1     25.0                                !iwtype initial, temp (C)
'        icon        guess          ctot          '
'h2o'      1        1.000d+00       1.000d+00
'h+'       1        0.6310d-8     -0.18618d-03
'ca+2'     1        0.2000d-2      0.1203d-02
'mg+2'     1        0.6500d-3      0.4814d-03
'na+'      1        0.2600d-2      0.2980d-02
'cl-'      1        0.3300d-2      0.1334d-02
'sio2(aq)' 1        0.1100d-2      0.????d-02
'hco3-'    1        0.3200d-2     0.16717d-02
'so4-2'    1        0.1200d-2      0.1020d-02
'k+'       1        0.2000d-3      0.1023d-03
'no3-'     1        1.100d-12      0.1387E-03
'*'        0         0.0            0.0
1     25.0                                !iwtype initial, temp (C)
'        icon        guess          ctot          '
'h2o'      1        1.000d+00       1.000d+00
'h+'       1        0.6310d-8     -0.18618d-03
'ca+2'     1        0.2000d-2      0.1203d-02
'mg+2'     1        0.6500d-3      0.4814d-03
'na+'      1        0.2600d-2      0.2980d-02
'cl-'      1        0.3300d-2      0.1334d-02
'sio2(aq)' 1        0.1100d-2      0.????d-02
'hco3-'    1        0.3200d-2     00.16717d-02
'so4-2'    1        0.1200d-2      0.1020d-02
'k+'       1        0.2000d-3      0.1023d-03
'no3-'     1        1.100d-12      0.1387E-03
'*'        0         0.0            0.0
'-----------------------------------------------------------------------'
'INITIAL MINERAL ZONES'
1
1
'mineral          vol.frac. msw33'
```

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5/31/06 Chemical inp (cont.)

```
chemical.inp                                                          5/30/2006

'quartz'              1.00000    1
.0E-00        300.        0
 '*'                  0.0      0
'-----------------------------------------------------------------------------'
'INITIAL gas ZONES'
1                                   !ngtype= number of gas zones
1                                   !igtype
'gas      partial pressure'    !at 25 C equil w/ atmosphere
'co2(g)'        3.163e-4
'*'                 0.0
'-----------------------------------------------------------------------------'
'Permeability-Porosity Zones: '
 1
 1
'perm law   a-par   b-par tcwM1'
    3    0.0000E+00    0.0000E+00
'-----------------------------------------------------------------------------'
'INITIAL SURFACE ADSORPTION ZONES'
0                    !ndtype= number of sorption zones
'zone       ad.surf.(m2/kg)  total ad.sites (mol/l)'
'-----------------------------------------if Sden=0 Kd store retardation factor'
'INITIAL LINEAR EQUILIBRIUM Kd ZONE'
1                                        !kdtpye=number of Kd zones
1                                        !idtype
'species   solid-density(Sden,kg/dm**3)  Kd(l/kg=mass/kg solid / mass/l'
'*'                 0.0                 0.0
'-----------------------------------------if Sden=0 Kd store retardation factor'
'INITIAL ZONES OF CATION EXCHANGE'
0                        !nxtype= number of exchange zones
'zone            ex. capacity'
'-----------------------------------------------------------------------------'
'end'
```

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Modeling Integrated Tests 5/31/06

Ambient Temperature, Pure Water, Quartz Simulation

This simulation will test the flow mesh and water saturation. The chemistry is very simple and involves dissolution of quartz. The existing input files will require some modification, described below.

Input modifications

Chemical.inp

'Primary Aqueous Species'
All species deleted except for h2O h+ SiO_2(aq)

'Minerals'
All minerals deleted except: quartz, SiO_2(amor), ~~and~~ QLM 5/31/06

'Initial + Boundary Water Types
Eliminated all aq species except H_2O, H^+, + SiO_2(aq)
The following parameters were ~~entered~~ changed for both initial + boundary water types QLM 5/31/06

	icon	guess	ctot
h+	3	1.0000d-7	1.000d-7
SiO2(aq)	1	QLM 5/31/06 ~~0.1100x10~~ 0.1100d-10	0.1000d-11

no other changes made to chemical.inp

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Input File Modifications (cont.)

Solute.inp

pointer of minerals for writing

deleted 18
replaced 12 w/ 1

no other changes made to solute.inp

Model Simulation

Ran treact_eos3 from command prompt.

Run stopped after reading flow.inp + solute.inp files

flow.out file revealed that the program was not reading the CONNE information from the MESH file that I created previously.

- resolved this problem by copying the ELEME + CONNE data from MESH and inserted it into flow.inp.

- Removed MESH file from the working directory.

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Modeling Integrated Tests 6/1/06
Model Simulation (cont.)

During an initial run TOUGHREACT reads the ELEME + CONNE information from the flow.inp file and creates a MESH file. (Then reads from the MESH file ~~prefer~~ JLM 6/1/06 preferentially over info. in flow.inp.) TOUGHREACT appears to replace zeros with blank spaces in some cases during the MESH file creation process. This apparently caused the programs to not recognize JLM 6/1/06 ~~some~~ JLM 6/1/06 element names that contained zeros instead of blanks.

Run tract_eos3 again

Run stopped after reading chemical.inp

Chemical.out revealed that the ther_ympR4a.dat thermodynamic data base does not contain SiO2(amor) Changed the mineral name to SiO2(am)_G that is in the above mentioned database

Chemical out contained the following message

GENERAL CHEMICAL SYSTEM
-> Thermodynamic database: ther_ympR4a.dat
Gas: CO2(g)
One or more components missing - stop

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Ambient Model Simulation (cont.)

The previous message was addressed by removing co2(g) from the chemical.inp file

It appears that hco3 (HCO_3^-) must be present as an aqueous component.

Ran react_eos3 again

Run appears to have completed normally

Review of flow.out indicates that the temperature is 239°C. (This is a remnant of the seed file used for this input

Made the following changes to flow.inp

PARAM

ELST = wdata — flag to obtain printout after ea. time step. Set to element name or wdata to read a list of element names below. Output to GASOBS.DAT. Following line contains integer value (3) for the number of element names. Followed by element names 1/line.

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Flow inp changes (cont.)

DEP(1) = 1.01325×10^5 P_g gas pressure (Pa)

DEP(2) = 0.1001×10^2 gas saturation (S_g + 10)
S_g + 10 flags code that
this is a 2-phase simulation,
liq + gas.

DEP(3) = 0.25×10^2 init. Temperature (°C)

note: the DEP(1), DEP(2), DEP(3) values have different definitions for different EOS units. These are defined above for the EOS3 unit and for the other units in the TOUGH2 ~~REACT~~ user's manual, section 6.
JLM 6/2/06

Ran react_eos3 again

Run appears to have executed to completion

Reviewed the flow out and figured out that the time steps in the printout are seconds, not days as I expected.

Changed the 15 entries in the "TIMES" section of flow.inp to their corresponding times in seconds from days JLM 6/2/06

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6/5/06 Modeling Integrated Tests
Ambient Model Simulation (cont.)
tract 9LM 6/5/06
Raw ~~tract~~ eos3

Review of flow out file indicates a problem w/ the run
- The program is outputting data for selected grid elements, not all grid elements, every 100 time steps.
  - It appears there might be a converge problem w/ this run. The runlog file is so big that I cannot open it on my disk top PC. The runlog for other successful runs is on the order of 100 kb or less

6/22/06 After making numerous changes to the flow.inp file, I was unable to resolve the above problem.

Decided to recreate the flow.inp file using Example problem 3 - Calcite deposition at YM as a seed file. This problem is similar to the integrated test problems in many ways. Many of the computation parameters are different from the original flow.inp that was created for this simulation.

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Modeling Integrated Tests 6/22/06

The new flow.inp file is presented below. The ELEME, CONNE, & GENER blocks are not shown because they are very large and ~~for~~ 9LM 6/22/06 did not change from previous flow.inp file.

```
flow.inp                                                                                    6/19/2006

# Integrated Tests 04/06: Quartz; pure water initial pH=7.00 T=25C (notebook:780)
# rebuilt flow.inp from example P3 in users manual.
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
rock1    1     2000.       .430  1.00E-11  1.00E-11  1.00E-11  2.70E+00     840.0
   0.0       0.0       0.0            0.0

REACT----1MOPR(20)-2----*----3----*----4----*----5----*----6----*----7----*----8
00012000
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*-123456789012345678901234----*----5----*----6----*----7----*----8
   39999    999900000000100020671003       2.14e-5      2.334        0.0
 0.00000E03.15576E09  1.00e+01 3.1536E04wdata       -9.806650
4
000 6
00066
00138
00282
    1.E-04
         1.01325E+05          0.10900E+020.2500000000000E+02

TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   15
  3.15E+05  3.15E+06  1.58E+07  2.21E+07  3.15E+07  3.15E+08  6.31E+08  9.46E+08
  1.26E+09  1.58E+09  1.89E+09  2.21E+09  2.52E+09  2.84E+09  3.15E+09

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    2    2    6

ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8    Real Vf
00001          rock10.1250E-030.2500E-02          0.2500E-010.2500E-01-.2500E-01
00013          rock10.1250E-030.0000E+00          0.2500E-010.2500E-01-.7500E-01
00025          rock10.1250E-030.0000E+00          0.2500E-010.2500E-01-.1250E+00
00037          rock10.1250E-030.0000E+00          0.2500E-010.2500E-01-.1750E+00
00049          rock10.1250E-030.0000E+00          0.2500E-010.2500E-01-.2250E+00
00061          rock10.1250E-030.0000E+00          0.2500E-010.2500E-01-.2750E+00
```


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Ran treact_eos3 using modified flow inp

Run completed execution, but failed to converge.
- Stopped ~~ab~~ JLM 6/22/06 after completing only a few time steps.

Contact Tianfu Xu, Lawrence Berkley lab, for ~~adv~~ 6/22/06 JLM advice on how to resolve the non-convergence problem

Tianfu reminded me that top & bottom boundary blocks are required when using EOS3 module to give the air some place to go when displaced by liquid. These blocks need to have volumes on the order of 1×10^{30}

Added a row of cells to the top & bottom of the existing flow mesh with volumes of 10^{32} m^3. This will ~~f~~ JLM 6/22/06 provide the vapor phase space to move, when displaced by liq

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Modeling Integrated Tests 7/31/06

The program is no longer having convergence problems.

I checked the liquid saturation (S_l) at the bottom of the grid (cell 282) and $S_l = 0.1075$. This value is close to the residual liq. sat (S_{lr}) = 0.1045.

I talked to Scott painter about the low S_l values. He suggested that I check the vertical S_l profile. If a gradient exists, then the problem is most like due to a boundary condition

layer		cell #	S_l
1		00006	0.3492
6		00066	0.3491
12	JLM 7/31/06	00ϕ138	0.3492
16		00186	0.3489
20		00234	0.3421
21		00246	0.3286
22		00258	0.2903
23		00270	0.1978
24 (bottom)		00282	0.1075

It appears that the bottom boundary is JLM 7/31/06 creating suction in the bottom portion of the grid.

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Increased the initial saturation of the bottom row of cells. This eliminated the observed draining of lower layers.

The simulation is now achieving liq. sat (S_l) results similar to equivalent run using MULTIFLO

Below is the first and last pages of the flow.inp file. The remainder of ELEME and section CONNE ~~Rome~~ JLM 7/31/06 are the same as previous versions of flow.inp.

Now that the flow characteristics in TOUGHREACT match up w/ MULTIFLO, I will begin to add more complex aqueous chemistry and mineralogy to the simulation and compare the results w/ MULTIFLO.

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Modeling Integrated Tests 7/31/06

```
flow.inp                                                                7/31/2006

# Integrated Tests: Qtz; pure water
# ROCK1 = Medium quartz sand
# init pH=7
# T=25C
# (notebook:780)
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*---
-8
rock1    2 2000.     0.430    0.1000E-100.1000E-100.1000E-10 2.700     840.0
                     0.350    0.0000
    7          0.627     .1045     1.000    0.000
   10          0.627     .10451.4800E-03   1.00e-7      1.00
topbd    2 2300.    0.2000    0.6026E-100.6026E-100.6026E-10 1.660
0.1000E+31
                         1.660  1.00
    1     0.2000    0.3000    0.7000    0.8000
    1                          1.000
botbd    2 2000.     0.430    0.1000E-100.1000E-100.1000E-10 2.700     840.0
                     0.350    0.0000
    7          0.627     .1045     1.000    0.000
    7          0.627     .10450.1480E-020.1000E+13   1.000
atmos    2 2300.    0.2000    0.0000E  30.0000E  30.0000E  3 1.660
0.1000E+31
                         0.0000
    1     0.2000    0.3000    0.7000    0.8000
    1                          1.000

REACT----1MOPR(20)-2----*----3----*----4----*----5----*----6----*----7----*---
-8
00012000
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*---
-8
PARAM----1----*-123456789012345678901234----*----5----*----6----*----7----*---
-8
   29999    999900000000000100020671005      2.14e-5     2.334        0.0
 0.00000E03.15576E09  1.00e+00 3.1536E04dummy       9.806650
    1.E-05
        0.101325E+06 0.1099000000000E+02 0.2500000000000E+02

TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*---
-8
   15
  3.15E+05  3.15E+06  1.58E+07  2.21E+07  3.15E+07  3.15E+08  6.31E+08
  9.46E+08
  1.26E+09  1.58E+09  1.89E+09  2.21E+09  2.52E+09  2.84E+09  3.15E+09

ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*---
-8   Real Vf
00001          rock10.1250E-030.2500E-02
0.2500E-010.2500E-01-.2500E-01
00013          rock10.1250E-030.0000E+00
0.2500E-010.2500E-01-.7500E-01
00025          rock10.1250E-030.0000E+00
0.2500E-010.2500E-01-.1250E+00
```


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7/31/06 Modeling Integrated Tests

```
flow.inp                                                                    7/25/2006

INCON -- INITIAL CONDITIONS FOR   54 ELEMENTS AT TIME  0.315360E+14
BT001   11    1            0.0
        0.101325E+06 0.1078500000000E+02 0.2500000000000E+02

ENDCY


MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*---
-8
    2    2    2    6

ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*---
-8
topbd    2 2300.    0.2000    0.6026E-100.6026E-100.6026E-10 1.660
0.1000E+31
                        1.660  1.00
    1     0.2000    0.3000    0.7000    0.8000
    1                         1.000
botbd    2 2300.    0.2800    0.5370E-170.5370E-170.5370E-17 1.350
0.1000E+31
                        1.5600 0.70
    7     0.3900              1.000
    7     0.3900              0.5800E-060.1000E+13 1.000
```

JLM 2/9/07

2/9/07 While working on the above flow.inp file I checked the TOUGH~~REACT~~ JLM 2/9/07 Users Guide and discovered that the ~~capp~~ JLM 2/9/07 capillary pressure function (ICP) = 10 is not defined but is used in example problems in the TOUGHREACT Users Guide

I contacted Tianfu Xu, LBNL, via email and received the following response.

This capillary pressure function is used as part of the THC modeling for the Yucca Mtn project. Follow up to make sure proper QA/QC was followed for this software change

INVENTOR SIGNATURE James L Myers PRINTED NAME DATE 2/9/07

DISCLOSED TO AND UNDERSTOOD BY PRINTED NAME DATE

Jim Myers

From: Tianfu Xu [Tianfu_Xu@lbl.gov]
Sent: Monday, July 03, 2006 3:33 PM
To: jmyers@cnwra.swri.edu
Subject: Re: Capillary Pressure ICP = 10

Jim,

ICP = 10 is a recent addtion for Yucca Mountain Project, was not described in standard TOUGH2 manual. I took a look the source code (in t2f.f file, see below). It's a modified van Genuchten Capillary pressure (Pc) function. For the original van Genuchten curve, when Sw is getting small Pc is fetting infinitive. Here using a linear extraplolation when Sw <= Swir.

Eric Sonnetthal and Yu-shu Wu knows the details. For further information, you can contact them.

-- Tianfu

```
   99 SLX=SL
c
c come here for linear extraplolation at Sw <= Swir
c    icp=10
c    cp(1,nmat)=m, v.G parameter
c    cp(2,nmat)=Swir
c    cp(3,nmat)=alpha, v.G. parameter
c    cp(4,nmat)=e, small number (defaul=1.e-5),
c            for Sw <= Swir+e using linear extrapolation
c    cp(5,nmat)=Sls
c
     IF(SLX.GE.CP(5,NMAT)) GOTO 1161
     IF(SLX.GT.(CP(2,NMAT)+cp(4,nmat))) then
```

Jim Myers wrote:

Tianfu,

I have been working through sample problem 4 and for the capillary pressure function for the first ROCK type the ICP value = 10. I do not see a description of this capillary pressure function in the TOUGH2 user's manual. Any help you can provide is appreciated. I have attached the flow.inp file for your information.

All of you help is greatly appreciated. If there is someone else that I can contact with flow questions please let me know.

Thank you,

Jim Myers
Geosciences and Engineering Division
Center for Nuclear Waste Regulatory Analyses
Southwest Research Institute
Ph: 210-522-6650
Fax: 210-522-6081

J L Myers

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 780

Document Date:	03/03/2006
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	■"Non-Sensitive" □ Sensitive □"Non-Sensitive - Copyright" □ Sensitive - Copyright
Date Generated:	03/03/2006
Operating System: (including version number)	Microsoft Windows
Application Used: (including version number)	
Media Type: (CDs, 3 ½, 5 1/4 disks, etc.)	1 CD
File Types: (.exe, .bat, .zip, etc.)	xls, dat, inp
Remarks: (computer runs, etc.)	Validation and Integrated test for TOUGHREACT Modeling