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ITOUGH2 V3.2

Verification and Validation Report

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1. Introduction

This report describes the Verification and Validation (V & V) test cases performed to qualify ITOUGH2 V3.2 in compliance with YMP-LBNL-QIP-SI.0, Rev. 3, Mod. 0. The testing of the software follows the V & V Plan as outlined in SCMS Form 3, Point 1, and addresses the functional requirements given in SCMS Form 2, Point 4.

The qualification of software related to ITOUGH2 is described in *Pruess et al.* [1996], *Wu et al.* [1996], and *Finsterle et al.* [1996].

The requirements are reproduced in Table 1.1. Additional information can be found in the user's manual [*Finsterle*, 1998].

Table 1.1. List of Requirements

#	Requirement	Section
	Fracture-matrix interface area reduced by:	
1.1	A constant	2.1.1
1.2	Upstream saturation	2.1.2
1.3	Upstream saturation times a constant	2.1.3
1.4	Upstream relative permeability	2.1.4
1.5	Upstream relative permeability times a factor	2.1.5
2	Free drainage boundary condition	2.2
3	Active Fracture Concept	2.3
4.1	Modification of Brooks-Corey capillary pressure function	2.4.1
4.2	Modification of van Genuchten capillary pressure function	2.4.2
5	New observation types SECONDARY and HEAT FLOW	2.5
6	New priorities in porosity definition	2.6
7	Adjusting array dimensions	2.7
8	Application control	2.8
9	Regression testing	2.9

ITOUGH2 V3.2 was installed in a directory `~/itough2v3.2` on a SUN ULTRA 1 workstation under UNIX Solaris 2. Instructions for installing ITOUGH2 can be found in file *read.me* and the user's manual.

This report is structured as follows: For each functional requirement, the corresponding design is described, which may include the mathematical model implemented in ITOUGH2 V3.2, if appropriate. Next, we discuss the test case or sequence of test cases performed to validate each requirement, followed by a description of the test results and their compliance with the acceptance criteria given in SCMS Form 3, Point 1.

2. Test Results

2.1 Fracture-Matrix Interface Area Reduction

There is evidence that fracture-matrix interaction in the unsaturated zone is reduced as a result of fracture coatings as well as preferential flow in the fractures as induced by flow instabilities (fingering) and small-scale heterogeneities. A number of options for reducing fracture-matrix interface area have been implemented for use in a dual-permeability flow simulation. Interface area reduction is applied to connections with a negative value for variable ISOT, which is provided in the CONNE block [Pruess, 1987]. Different modifiers are used depending on the value of ISOT and MOP (8) as summarized in Table 2.1.1.

Table 2.1.1. Option for Reducing Fracture-Matrix Interface Area

ISOT	MOP (8)	Interface area reduction factor a_{fm}
1, 2, 3	any	No interface area reduction, i.e., $a_{fm} = 1$
negative	1	$a_{fm} = RP(6, NMAT)$
-1, -2, -3	0	$a_{fm} = S_{\beta}$
	2	$a_{fm} = S_{\beta} \cdot RP(7, NMAT)$
-4, -5, -6	0	$a_{fm} = k_{r\beta}$
	2	$a_{fm} = k_{r\beta} \cdot RP(7, NMAT)$
-10, -11, -12	0	$a_{fm} = S_e^{1+\gamma}$ (see Section 2.3)

a_{fm}	:	Fracture-matrix interface area reduction factor.
S_{β}	:	For flow of phase β , upstream saturation of phase β .
$k_{r\beta}$:	For flow of phase β , upstream relative permeability of phase β .
$RP(6, NMAT)^{\#}$:	6th parameter of rel. perm. function of upstream element.
$RP(7, NMAT)^{\#}$:	7th parameter of rel. perm. function of upstream element.
$\#$:	If zero (i.e., not specified), reset to one.

Figure 2.1.1 shows the pseudo-code implemented for the interface area reduction calculation, revealing the control logic.

```

afm:=1
if ISO negative then
  determine material number NMAT of upstream gridblock
  if ISO=-1, -2, or -3 then
    afm:=upstream saturation
  else if ISO=-4, -5, or -6 then
    afm:=upstream relative permeability
  else if ISO=-10, -11, or -12 then
    afm:=Equation (2.3.6)
  end if
  if MOP(8)=1 then
    afm:=RP(6,NMAT)
  else if MOP(8)=2 then
    afm=afm*RP(7,NMAT)
  end if
end if
area:=area*afm

```

Figure 2.1.1. Pseudo-code for interface area reduction.

To validate whether the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the corresponding factor described in Table 2.1.1, a one-dimensional, dual-permeability fracture-matrix model was developed with constant infiltration at the top and constant pressure and saturation at the bottom. The generic TOUGH2 input file is shown in Figure 2.1.2. The model has two layers, each layer with its own set of fracture and matrix properties. Note that the first four entries in block CONNE represent the connections between the fracture and matrix gridblocks, which will be subjected to interface area reduction. The different options are implemented by changing MOP(8), ISO, and AREA as described in the following sections.

Because of successful regression testing (see Section 2.9), the Run B simulations described below can be performed using either standard TOUGH2 or ITOUGH2 in forward mode.

```

Fracture-Matrix Interface Area Reduction
ROCKS---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
FRAC1  2  2000.0  0.10  1.0E-12  1.0E-12  1.0E-12  2.0  900.0
      7  0.5000  0.0100  1.0000  0.01  0.1
      7  0.5000  0.0100  1.000E-04  1.000
MATR1  2  2000.0  0.10  1.0E-17  1.0E-17  1.0E-17  2.0  900.0
      7  0.2500  0.1000  1.0000  0.01  0.1
      7  0.2500  0.1000  1.000E-05  1.000
FRAC2  2  2000.0  0.10  1.0E-12  1.0E-12  2.0  900.0
      7  0.5000  0.0100  1.0000  0.01  0.1
      7  0.5000  0.0100  1.000E-03  1.000
MATR2  2  2000.0  0.10  1.0E-16  1.0E-16  2.0  900.0
      7  0.2000  0.1500  1.0000  0.01  0.1
      7  0.2000  0.1500  1.000E-06  1.000

START---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
PARAM  123456789012345678901234
-39999 9999000000110000000400003000
1.000E-05 1.0E+06 9.81
      0.8

ELEME---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
F  1  10.1000E-010.1000E-01  -.5000E+00
M  1  20.1000E+010.1000E+01  -.5000E+00
F  2  10.1000E-010.0000E+00  -.1500E+01
M  2  20.1000E+010.0000E+00  -.1500E+01
F  3  30.1000E-010.0000E+00  -.2500E+01
M  3  40.1000E+010.0000E+00  -.2500E+01
F  4  30.1000E-010.0000E+00  -.3500E+01
M  4  40.1000E+010.0000E+00  -.3500E+01
F  5  3-.1000E-010.1000E-01  -.4500E+01
M  5  4-.1000E+010.1000E+01  -.4500E+01

CONNE---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
F  1M  1  -10.0000E+000.5000E+000.1000E+01
F  2M  2  -10.0000E+000.5000E+000.1000E+01
F  3M  3  -10.0000E+000.5000E+000.1000E+01
F  4M  4  -10.0000E+000.5000E+000.1000E+01
M  1M  2  30.5000E+000.5000E+000.1000E+010.1000E+01
M  2M  3  30.5000E+000.5000E+000.1000E+010.1000E+01
M  3M  4  30.5000E+000.5000E+000.1000E+010.1000E+01
M  4M  5  30.5000E+000.5000E+000.1000E+010.1000E+01
F  1F  2  30.5000E+000.5000E+000.1000E-010.1000E+01
F  2F  3  30.5000E+000.5000E+000.1000E-010.1000E+01
F  3F  4  30.5000E+000.5000E+000.1000E-010.1000E+01
F  4F  5  30.5000E+000.5000E+000.1000E-010.1000E+01

GENER---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
F  1  COM1 1.0000E-07

INCON---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
M  5
0.99
F  5
0.02

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

```

Figure 2.1.2. Generic TOUGH2 input file for validating fracture-matrix interface area reduction.

2.1.1.1 Interface Area Reduced by a Constant

To confirm that the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the constant provided through TOUGH2 input variable RP(6,NMAT), the following two runs were performed:

Run A: Steady-state simulation with geometric interface area, using negative values for ISOT, setting MOP(8)=1, and setting RP(6,NMAT)=0.01 for all rock types. The input file is named *vvFMIA*; it is shown in Figure 2.1.2.

Run B: Steady-state simulation with interface areas reduced to 1% of their geometric values and positive ISOT. The input file is named *vvFMIB*; the CONNE block is reproduced in Figure 2.1.1.1.

Because of limited accuracy in specifying interface areas in the TOUGH2 input file, there may be slight differences in the two results. However, for the values chosen here, both runs should yield identical results.

The following command lines were used to run the test cases:

```
itough2 -v3.2 vvFM1A 9 &
itough2 -v3.2 vvFM1B 9 &
```

Inspection of the two output files *vvFMIA.out* and *vvFMIB.out* confirms that identical results were obtained, fulfilling Requirement 1.1.

CONNE	1	2	3	4	5	6	7	8
F 1M	1			10.0000E+000	.5000E+000	.1000E-01		
F 2M	2			10.0000E+000	.5000E+000	.1000E-01		
F 3M	3			10.0000E+000	.5000E+000	.1000E-01		
F 4M	4			10.0000E+000	.5000E+000	.1000E-01		
M 1M	2			30.5000E+000	.5000E+000	.1000E+010	.1000E+01	
M 2M	3			30.5000E+000	.5000E+000	.1000E+010	.1000E+01	
M 3M	4			30.5000E+000	.5000E+000	.1000E+010	.1000E+01	
M 4M	5			30.5000E+000	.5000E+000	.1000E+010	.1000E+01	
F 1F	2			30.5000E+000	.5000E+000	.1000E-010	.1000E+01	
F 2F	3			30.5000E+000	.5000E+000	.1000E-010	.1000E+01	
F 3F	4			30.5000E+000	.5000E+000	.1000E-010	.1000E+01	
F 4F	5			30.5000E+000	.5000E+000	.1000E-010	.1000E+01	

Figure 2.1.1.1. Block CONNE of file *vvFMIB*, showing positive values for variable ISOT and interface areas reduced to 1% of the values shown in Figure 2.1.2.

2.1.2 Interface Area Reduced by Upstream Saturation

To confirm that the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the saturation of the upstream gridblock, the following two runs were performed:

Run A: Steady-state simulation with geometric interface area, setting ISOT=-1, and MOP(8)=0. The input file is named *vvFM2A*; it is identical to the file shown in Figure 2.1.2, with the exception of MOP(8).

Run B: Steady-state simulation with interface areas specified directly in block CONNE, reduced by the steady-state upstream saturation calculated in Run A. The input file is named *vvFM2B*.

The results of the two runs are expected to be slightly different because (1) there is limited accuracy in specifying interface areas in the TOUGH2 input file, and (2) while the interface area available for flow changes with saturation (and thus with time) in Run A, the reduced value is fixed throughout Run B. This difference leads to a different system development as it evolves from its initial state towards steady-state conditions, with different time steps taken, different total simulation times to reach steady state, and different number of iterations, leading to different round-off and time-discretization errors. Nevertheless, the results at steady-state are expected to be very similar, with the maximum difference in any output variable being less than 0.1%.

The following command line was used for Run A:

```
itough2 -v3.2 vvFM2A 9 &
```

The saturations as written to the SAVE file *vvFM2A.sav* (see Figure 2.1.2.1) are used as reduction factors of the interface areas of the first four connections specified in the CONNE block of file *vvFM2B* as shown in Figure 2.1.2.2. At steady state, flow is from the fractures into the matrix, making the fracture gridblocks the upstream gridblocks.

```

INCON -- INITIAL CONDITIONS FOR 10 ELEMENTS AT TIME 0.429497E+16
F 1 0.10000000E+00
0.4338920874502E+00 0.00000000000000E+00
M 1 0.10000000E+00
0.8921064332228E+00 0.00000000000000E+00
F 2 0.10000000E+00
0.6098054293383E+00 0.00000000000000E+00
M 2 0.10000000E+00
0.8960659745952E+00 0.00000000000000E+00
F 3 0.10000000E+00
0.2750228155389E+00 0.00000000000000E+00
M 3 0.10000000E+00
0.9881525567958E+00 0.00000000000000E+00
F 4 0.10000000E+00
0.1754130794552E+00 0.00000000000000E+00
M 4 0.10000000E+00
0.9890779950707E+00 0.00000000000000E+00
F 5 0.10000000E+00
0.2000000000000E-01 0.00000000000000E+00
M 5 0.10000000E+00
0.9900000000000E+00 0.00000000000000E+00
+++
34 89 4 0.10000000E-04 0.42949673E+16

```

Figure 2.1.2.1. File *vvFM2A.sav*, showing steady-state saturations obtained in Run A.

```

CONNE---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
F 1M 1 10.0000E+00.5000E+00.43389087
F 2M 2 10.0000E+00.5000E+00.60980543
F 3M 3 10.0000E+00.5000E+00.27502282
F 4M 4 10.0000E+00.5000E+00.17541308
M 1M 2 30.5000E+00.5000E+00.1000E+010.1000E+01
M 2M 3 30.5000E+00.5000E+00.1000E+010.1000E+01
M 3M 4 30.5000E+00.5000E+00.1000E+010.1000E+01
M 4M 5 30.5000E+00.5000E+00.1000E+010.1000E+01
F 1F 2 30.5000E+00.5000E+00.1000E-010.1000E+01
F 2F 3 30.5000E+00.5000E+00.1000E-010.1000E+01
F 3F 4 30.5000E+00.5000E+00.1000E-010.1000E+01
F 4F 5 30.5000E+00.5000E+00.1000E-010.1000E+01

```

Figure 2.1.2.2. Block CONNE of file *vvFM2B*, showing interface areas reduced by the fracture saturations shown in Figure 2.1.2.1.

The following command line was used for Run B:

```
itough2 -v3.2 vvFM2B 9 &
```

Inspection of the two output files *vvFM2A.out* and *vvFM2B.out* confirms that identical results were obtained, fulfilling Requirement 1.2.

2.1.3 Interface Area Reduced by Upstream Saturation Times a Constant

To confirm that the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the saturation of the upstream gridblock times the factor provided through variable RP(7,NMAT), the following two runs were performed:

Run A: Steady-state simulation with geometric interface area, setting ISOT=-1, and MOP(8)=2, and RP(7,NMAT)=0.1 for all rock types. The input file is named *vvFM3A*; it is identical to the file shown in Figure 2.1.2, with the exception of MOP(8).

Run B: Steady-state simulation with interface areas specified directly in block CONNE, reduced by the steady-state upstream saturation calculated in Run A times 0.1. The input file is named *vvFM3B*.

The results at steady-state are expected to be very similar, with the maximum difference in any output variable being less than 0.1%.

The following command line was used for Run A:

```
itough2 -v3.2 vvFM3A 9 &
```

The saturations as written to the SAVE file *vvFM3A.sav* (see Figure 2.1.3.1) are used as reduction factors of the interface areas specified for the first four connections in the CONNE block of file *vvFM3B* as shown in Figure 2.1.3.2. The interface areas are further reduced by 0.1, which is the factor specified in RP(7,NMAT) of Run A. At steady state, flow is from the fractures into the matrix, making the fracture gridblocks the upstream gridblocks.

```

INCON -- INITIAL CONDITIONS FOR 10 ELEMENTS AT TIME 0.429497E+16
F 1 0.10000000E+00
0.4376531245338E+00 0.00000000000000E+00
M 1 0.10000000E+00
0.8357579578799E+00 0.00000000000000E+00
F 2 0.10000000E+00
0.6175860651419E+00 0.00000000000000E+00
M 2 0.10000000E+00
0.8436032656234E+00 0.00000000000000E+00
F 3 0.10000000E+00
0.2911632608216E+00 0.00000000000000E+00
M 3 0.10000000E+00
0.9878238253713E+00 0.00000000000000E+00
F 4 0.10000000E+00
0.1852263062714E+00 0.00000000000000E+00
M 4 0.10000000E+00
0.9889180282040E+00 0.00000000000000E+00
F 5 0.10000000E+00
0.2000000000000E-01 0.00000000000000E+00
M 5 0.10000000E+00
0.9900000000000E+00 0.00000000000000E+00
+++
35 89 4 0.10000000E-04 0.42949673E+16

```

Figure 2.1.3.1. File *vvFM3A.sav*, showing steady-state saturations obtained in Run A.

```

CONNE---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
F 1M 1 10.0000E+000.5000E+000.04376531
F 2M 2 10.0000E+000.5000E+000.06175871
F 3M 3 10.0000E+000.5000E+000.02911633
F 4M 4 10.0000E+000.5000E+000.01852263
M 1M 2 30.5000E+000.5000E+000.1000E+010.1000E+01
M 2M 3 30.5000E+000.5000E+000.1000E+010.1000E+01
M 3M 4 30.5000E+000.5000E+000.1000E+010.1000E+01
M 4M 5 30.5000E+000.5000E+000.1000E+010.1000E+01
F 1F 2 30.5000E+000.5000E+000.1000E-010.1000E+01
F 2F 3 30.5000E+000.5000E+000.1000E-010.1000E+01
F 3F 4 30.5000E+000.5000E+000.1000E-010.1000E+01
F 4F 5 30.5000E+000.5000E+000.1000E-010.1000E+01

```

Figure 2.1.3.2. Block CONNE of file *vvFM3B*, showing interface areas reduced by 10% of the fracture saturations shown in Figure 2.1.3.1.

The following command line was used for Run B:

```
itough2 -v3.2 vvFM3B 9 &
```

Inspection of the two output files *vvFM3A.out* and *vvFM3B.out* confirms that identical results were obtained, fulfilling Requirement 1.3.

2.1.4 Interface Area Reduced by Upstream Relative Permeability

To confirm that the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the relative permeability of the upstream gridblock, the following two runs were performed:

Run A: Steady-state simulation with geometric interface area, setting ISOT=-4, and MOP(8)=0. The input file is named *vvFM4A*; it is identical to the file shown in Figure 2.1.2, with the exception of MOP(8) and ISOT for the first four connections.

Run B: Steady-state simulation with interface areas specified directly in block CONNE, reduced by the steady-state upstream relative permeability calculated in Run A. The input file is named *vvFM4B*.

The results at steady-state are expected to be very similar, with the maximum difference in any output variable being less than 0.1%.

The following command line was used for Run A:

```
itough2 -v3.2 vvFM4A 9 &
```

The liquid relative permeabilities as written to the TOUGH2 output file *vvFM4A.out* (see Figure 2.1.4.1) are used as reduction factors of the interface areas of the first four connections specified in the CONNE block of file *vvFM4B* as shown in Figure 2.1.4.2. At steady state, flow is from the fractures into the matrix, making the fracture gridblocks the upstream gridblocks.

2.1.5 Interface Area Reduced by Upstream Relative Permeability Times a Constant

To confirm that the interface area available for fluid flow between two adjacent gridblocks is reduced from its geometric value by the relative permeability of the upstream gridblock times the factor provided through variable $RP(7,NMAT)$, the following two runs were performed:

Run A: Steady-state simulation with geometric interface area, setting $ISOT=-4$, $MOP(8)=2$, and $RP(7,NMAT)=0.1$ for all rock types. The input file is named *vvFM5A*; it is identical to the file shown in Figure 2.1.2, with the exception of $MOP(8)$ and $ISOT$ for the first four connections.

Run B: Steady-state simulation with interface areas specified directly in block $CONNE$, reduced by 10% of the steady-state upstream liquid saturation calculated in Run A. The input file is named *vvFM5B*.

The results at steady-state are expected to be very similar, with the maximum difference in any output variable being less than 0.1%.

The following command line was used for Run A:

```
itough2 -v3.2 vvFM5A 9 &
```

The liquid relative permeabilities as written to the TOUGH2 output file *vvFM5A.out* (see Figure 2.1.5.1) are used as reduction factors of the interface area specified in the $CONNE$ block of file *vvFM5B* as shown in Figure 2.1.5.2. The interface areas are further reduced by 0.1, the factor specified in variable $RP(7,NMAT)$ in Run A. At steady state, flow is from the fractures into the matrix, making the fracture gridblocks the upstream gridblocks.

2.2 Free Drainage Boundary Condition

A free drainage boundary condition for liquid flow is implemented, in which gravity is the only driving force, i.e., (capillary) pressure gradients are ignored across the interface to a boundary gridblock. This type of boundary condition comes into effect at each connection, in which one of the gridblocks belongs to rock type DRAIN.

To test whether the free drainage boundary condition is correctly implemented, one-dimensional, gravity-driven, unsaturated flow is calculated with a free drainage boundary condition at the bottom of the column. If the resulting steady-state saturation profile is uniform and not affected by the capillary pressure gradient to the boundary gridblock, the implementation is considered correct.

The TOUGH2 input file is shown in Figure 2.2.1. Note that the last element is inactive (negative volume) and associated with rock type DRAIN.

The following command line was used for Run B:

```
itough2 -v3.2 vvFDBC 9 &
```

The steady-state solution (TOUGH2 output file *vvFDBC.out*) is shown in Figure 2.2.2. Note that the boundary gridblock would act as a capillary barrier, leading to a saturation buildup and thus nonuniform saturation profile. However, as a result of the newly implemented free drainage boundary condition, the saturation profile is uniform, fulfilling Requirement 2.

```
Free drainage boundary condition
ROCKS-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
FRACT      2      2000.0      0.10      1.0E-12      1.0E-12      1.0E-12      2.0      900.0

      7      0.5000      0.0100      1.0000
      7      0.5000      0.0100      1.000E-04      1.0000
DRAIN      2      2000.0      0.10      1.0E-12      1.0E-12      1.0E-12      2.0      900.0

      7      0.5000      0.0100      1.0000
      7      0.5000      0.0100      1.000E-04      1.0000

START-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
PARAM      123456789012345678901234
-39999      9999000000110000000400003000
1.000E-05      1.0E+06      9.81

      0.5
MULTI-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
      1      1      1      6

ELEME-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
F      1      10.1000E+000.1000E-01      -.5000E+01
F      2      10.1000E+000.0000E+00      -.1500E+02
F      3      10.1000E+000.0000E+00      -.2500E+02
F      4      10.1000E+000.0000E+00      -.3500E+02
F      5      2-.1000E+000.1000E-01      -.4500E+02

CONNE-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
F      1F      2      30.5000E+010.5000E+010.1000E-010.1000E+01
F      2F      3      30.5000E+010.5000E+010.1000E-010.1000E+01
F      3F      4      30.5000E+010.5000E+010.1000E-010.1000E+01
F      4F      5      30.5000E+010.5000E+010.1000E-010.1000E+01

GENER-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
F      1      COM1 1.0000E-07

ENDCY-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
```

Figure 2.2.1. TOUGH2 input file *vvFDBC* for free drainage boundary problem.

2.3 Active Fracture Concept

There is evidence that only a portion of the connected fracture network conducts water under unsaturated conditions. The fractures contributing to liquid flow are referred to as “active fractures”. The Active Fracture Concept (AFC) was developed by *Liu et al.* [1998] to describe gravity-dominated, non-equilibrium, preferential liquid flow in fractures, which is expected to be similar to fingering in unsaturated porous media. AFC is based on the hypothesis that (1) the number of active fractures is small compared with the total number of connected fractures, (2) the number of active fractures within a gridblock is large so that the continuum approach is valid, and (3) the fraction of active fractures, f_a , is related to water flux and equals one for a fully saturated system, and zero if the system is at residual saturation. The following power function of effective liquid saturation, S_e , fulfills these conditions:

$$f_a = S_e^\gamma \quad (2.3.1)$$

Here, γ is a positive constant depending on properties of the fracture network, and S_e is the effective liquid saturation given by

$$S_e = \frac{S_l - S_{lr}}{1 - S_{lr}} \quad (2.3.2)$$

Capillary pressure and relative permeability functions are modified to account for the fact that the effective saturation in the active fractures, S_{ea} , is larger than the effective saturation of the total fracture continuum:

$$S_{ea} = \frac{S_e}{f_a} = S_e^{1-\gamma} \quad (2.3.3)$$

Using the van Genuchten model, capillary pressure and liquid relative permeability are given, respectively, by

$$p_c = -\frac{1}{\alpha} \left[S_e^{(\gamma-1)/m} - 1 \right]^{1/n} \quad (2.3.4)$$

and

$$k_{rl} = S_e^{(1+\gamma)/2} \left\{ 1 - \left[1 - S_e^{(1-\gamma)/m} \right]^m \right\}^2 \quad (2.3.5)$$

The fracture-matrix interface area reduction factor (see Section 2.1) is given by

$$a_{fm} = S_e^{1+\gamma} \quad (2.3.6)$$

The AFC is invoked by selecting $\gamma > 0$, which is provided as an additional parameter of the standard van Genuchten model (ICP=7) through variable CP(6,NMAT). Fracture-matrix interface area reduction according to Eq. (2.3.6) is invoked by selecting ISOT between -10 and -12.

The AFC is implemented by modifying the capillary pressure and relative permeability functions. The implementation is tested by directly comparing the values (i.e., saturation, capillary pressure, and relative permeability) given in the TOUGH2 output file with the ones calculated using Eqs. (2.3.2) through (2.3.5).

The TOUGH2 input file shown in Figure 2.3.1 is used for testing of the AFC as well as other requirements (see below).

```

TOUGH2 input file for V&V of:
(1) Active Fracture Concept
(2) Modified Brooks-Corey function
(3) Modified van Genuchten function
(4) New observation type SECONDARY
(5) New observation type HEAT FLOW
(6) Handling of porosity
(7) ITOUGH2 application control

ROCKS-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
AFC          2      2000.0      0.1      1.0E-12      1.0E-12      1.0E-12      2.0      900.0
          7          0.5000      0.1000      1.000
          7          0.5000      0.1000      0.001      1.0E+10      1.0      0.5
BC          2      2000.0      0.2      1.0E-12      1.0E-12      1.0E-12      2.0      900.0
          10          0.3000      0.1000
          10          2.0000      1000.0      0.100
VG          2      2000.0      0.3      1.0E-12      1.0E-12      1.0E-12      2.0      900.0
          11          0.3000      0.1000
          11          3.0000      1000.0      0.100
BC2         2      2000.0      0.2      1.0E-12      1.0E-12      1.0E-12      2.0      900.0
          10          0.2000      0.1000      1.0
          10          2.0000      1000.0      7000.0
VG2         2      2000.0      0.3      1.0E-12      1.0E-12      1.0E-12      2.0      900.0
          11          0.2000      0.1000      1.0
          11          3.0000      1000.0      7000.0

PARAM-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
3 1      110000801000000000400001000
          1.0
          1.0E5
          10.3
          20.0
MULTI-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
2 3      2      6
ELEM-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
ELM 1          AFC          0.1
ELM 2          BC          0.1
ELM 3          VG          0.1

CONNE-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
ELM 1ELM 2          -10      0.05      0.05      0.10
ELM 2ELM 3          1      0.05      0.05      0.10

START-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
INCON-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
ELM 1          0.4
ELM 2          1.1E5          0.5          10.3          50.0
          1.0E5          10.3          20.0

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

```

Figure 2.3.1. TOUGH2 input file *vv* used for testing of Active Fracture Concept, modified Brooks-Corey and van Genuchten functions, newly implemented observation types, and handling of porosity.

The parameters used for the AFC as given in the TOUGH2 input file (see Figure 2.3.1) are summarized in Table 2.3.1.

Table 2.3.1. Parameters of AFC

Parameter	TOUGH2 Parameter	Value
S_{lr}	RP(2), CP(2)	0.10
γ	CP(6)	0.50
α	CP(3)	0.001
m	RP(1), CP(1)	0.50
$n = 1 / (1 - m)$	-	2.00
k	PER(1)	1.0E-12
A	AREAX	0.10
d_1, d_2	DEL1, DEL2	0.05

Figure 2.3.2 shows an excerpt from the TOUGH2 output file *vv.out*, which is obtained by running the problem with the following command line:

```
tough2 -v 3.2 vv 3 &
```

The liquid saturation in gridblock “ELM 1”, to which the AFC characteristic curves are assigned, is 0.69998. Inserting this value along with the parameters of Table 2.3.1. into Eqs. (2.3.2), (2.3.4), and (2.3.5) yields the following capillary pressure and liquid relative permeability:

$$S_e = \frac{0.69998 - 0.1}{1 - 0.1} = 0.66664$$

$$p_c = -\frac{1}{0.001} \left[0.66664^{(0.5-1)/0.5} - 1 \right]^{1/2.0} = -707.15$$

$$k_{rl} = 0.66664^{(1+0.5)/2} \left\{ 1 - \left[1 - 0.66664^{(1-0.5)/0.5} \right]^{0.5} \right\}^2 = 0.13177$$

These values are consistent with the ones reported in the TOUGH2 output file (Figure 2.3.2).

The fracture-matrix interface area reduction factor (see Section 2.1) is given by Eq. (2.3.6):

$$a_{fm} = 0.66664^{1+0.5} = 0.5443$$

Applying Darcy’s law between gridblocks “ELM 2” and “ELM 1” yields:

$$\begin{aligned}
q_{ELM2-ELM1} &= -k \cdot A \cdot a_{jm} \frac{k_{rl}}{\mu_l} \rho_l \left(\frac{P_{ELM1} - P_{ELM2}}{d_1 + d_2} \right) \\
&= -10^{-12} \cdot 0.1 \cdot 0.5443 \frac{0.13177}{5.4418 \cdot 10^{-4}} 988.07 \left(\frac{1.0704 \cdot 10^5 - 1.0002 \cdot 10^5}{0.05 + 0.05} \right) \\
&= -9.142 \cdot 10^{-4} \text{ kg / s}
\end{aligned}$$

which is consistent with the liquid flux at the first connection. These results fulfill Requirement 3.

```

TOUGH2 input file for V&V of:
      OUTPUT DATA AFTER ( 1, 3)-2-TIME STEPS                                THE TIME IS 0.11574E-04 DAYS
#####
TOTAL TIME   KCYC   ITER  ITERC   KON      DX1M      DX2M      DX3M      MAX. RES.   NER    KER      DELTEX
0.10000E+01   1     3     3     2      0.22506E+04 0.23491E-04 0.11000E-02 0.24540E-08 1     2     0.10000E+01
#####
ELEM.  INDEX   P          T          SG          SL          XAIRG      XAIRL      PSAT        PCAP        DG          DL
      (PA)      (DEG-C)
ELM 1    1 0.10775E+06 0.49999E+02 0.30002E+00 0.69998E+00 0.92531E+00 0.15337E-04 0.12335E+05 -0.70715E+03 0.11114E+01 0.98807E+03
ELM 2    2 0.10134E+06 0.20001E+02 0.29999E+00 0.70001E+00 0.98551E+00 0.15914E-04 0.23367E+04 -0.13229E+04 0.11936E+01 0.99832E+03
ELM 3    3 0.10005E+06 0.20000E+02 0.29999E+00 0.70001E+00 0.98533E+00 0.15707E-04 0.23366E+04 -0.10956E+04 0.11783E+01 0.99832E+03
#####
      TOUGH2 input file for V&V of:
0      ELEM1  ELEM2  INDEX   FLOH      FLOH/FLOF      FLOF      FLO(GAS)      KCYC = 1 - ITER = 3 - TIME = 0.10000E+01
      (W)      (J/KG)      (KG/S)      (KG/S)      FLO(LIQ.)      VEL(GAS)      VEL(LIQ.)
      (KG/S)      (M/S)      (M/S)
      ELM 1  ELM 2    1 -0.35311E+03 0.28499E+06 -0.12390E-02 -0.32429E-03 -0.91476E-03 -0.24313E-01 -0.60749E-04
      ELM 2  ELM 3    2 -0.18307E+02 0.85196E+05 -0.21488E-03 -0.52482E-05 -0.20963E-03 -0.24428E-03 -0.49995E-05
#####
      TOUGH2 input file for V&V of:
ELEM.  INDEX  X1          X2          X3          DX1          DX2          DX3      KCYC = 1 - ITER = 3 - TIME = 0.10000E+01
      K(GAS)      K(LIQ.)      H(GAS)      H(LIQ.)
      (J/KG)      (J/KG)
ELM 1    1 0.10775E+06 0.10300E+02 0.49999E+02 -0.22506E+04 0.23491E-04 -0.55264E-03 0.86822E+00 0.13178E+00 0.31337E+06 0.20934E+06
ELM 2    2 0.10134E+06 0.10300E+02 0.20001E+02 0.13411E+04 -0.12058E-04 0.11000E-02 0.61718E-01 0.19755E+00 0.13416E+06 0.83959E+05
ELM 3    3 0.10005E+06 0.10300E+02 0.20000E+02 0.49100E+02 -0.69924E-05 0.33025E-05 0.24311E+00 0.13583E+00 0.13462E+06 0.83954E+05
#####

```

Figure 2.3.2. Excerpt from TOUGH2 output file *vv.out* showing saturation, capillary pressure, and relative liquid permeability of element ELM 1, to which the Active Fracture Concept is applied.

2.4 Modification to Capillary Pressure Functions

Modified versions of the Brooks-Corey and van Genuchten models [Luckner *et al.*, 1989] were implemented. In order to prevent the capillary pressure from decreasing towards negative infinity as the effective saturation approaches zero, a linear function is used for saturations S_l below a certain value ($S_{lr} + \varepsilon$), where ε is a small number. The slope of the linear extrapolation is identical with the slope of the capillary pressure curve at $S_l = S_{lr} + \varepsilon$. Alternatively, the capillary pressure is prevented from becoming more negative than $-p_{c,\max}$.

The correct implementation is checked by visual inspection of the capillary pressure curves near residual saturation. Capillary pressure vs. saturation data in the range $0 \leq S_l \leq 1$ are written to a separate file for plotting when ITOUGH2 command `>>> CHARACTERISTIC` is given. The plot file `vvi_ch.tec` was created using the following command line:

```
itough2 -v 3.2 vvi vv 3 &
```

2.4.1 Modification to Brooks-Corey Capillary Pressure Function

The modified Brooks-Corey model is invoked by setting both `IRP` and `ICP` to 10. The model is described by the following set of equations (the input parameters are listed in Table 2.4.1.1):

$$S_{ec} = \frac{S_l - S_{lrc}}{1 - S_{lrc}} \quad (2.4.1.1a)$$

$$S_{ek} = \frac{S_l - S_{lrk}}{1 - S_{lrk} - S_{gr}} \quad (2.4.1.1b)$$

$$p_c = -p_e (S_{ec})^{-1/\lambda} \quad \text{for } S_l \geq (S_{lrc} + \varepsilon) \quad (2.4.1.2a)$$

$$p_c = -p_e \left(\frac{\varepsilon}{1 - S_{lrc}} \right)^{-1/\lambda} - \frac{p_e}{\lambda} \left(\frac{\varepsilon}{1 - S_{lrc}} \right)^{-\frac{1-\lambda}{\lambda}} (S_l - S_{lrc} - \varepsilon) \quad \text{for } S_l < (S_{lrc} + \varepsilon) \quad (2.4.1.2b)$$

$$p_c \geq -p_{c,\max} \quad (2.4.1.3)$$

$$k_{rl} = S_{ek}^{\frac{2-3\lambda}{\lambda}} \quad (2.4.1.4a)$$

$$k_{rg} = (1 - S_{ek})^2 \left(1 - S_{ek}^{\frac{2+\lambda}{\lambda}} \right) \quad (2.4.1.4b)$$

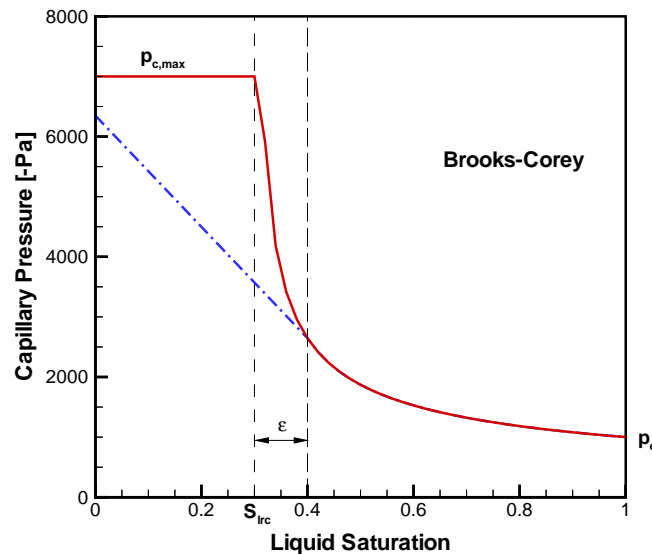
$$k_{rg} = 1 - k_{rl} \quad (2.4.1.4c)$$

Table 2.4.1.1. Input Parameters for Modified Brooks-Corey Model

Parameter	Variable	Description
<i>IRP</i>	10	select Brooks-Corey relative permeability model
<i>RP(1)</i>	S_{lrk}	residual liquid saturation for relative permeability functions
<i>RP(2)</i>	S_{gr}	residual gas saturation
<i>RP(3)</i>	(flag)	if zero, use (2.4.1.4b), otherwise (2.4.1.4c)
<i>ICP</i>	10	select Brooks-Corey capillary pressure model
<i>CP(1)</i>	λ	pore size distribution index
<i>CP(2)</i>	p_e	gas entry pressure [Pa]
<i>CP(3)</i>	ε or $p_{c,max}$	if $CP(3) = 0$ then $p_{c,max} = 10^{50}$, $\varepsilon = -1$ if $0 < CP(3) < 1$ use linear model (2.4.1.2b) for $S_l < S_{lr} + \varepsilon$ if $CP(3) \geq 1$, then $p_{c,max} = CP(3)$, $\varepsilon = -1$
<i>CP(6)</i>	S_{lrc}	if zero, then $S_{lrc} = S_{lrk}$

Figure 2.4.1.1 shows two modified Brooks-Corey capillary pressure functions. The first one, shown by the solid line, was produced with $CP(3) = p_{c,max} = 7000$, limiting the capillarity to values larger than $p_c = -7000$ Pa. The second curve, shown by the broken line, was produced with $CP(3) = \varepsilon = 0.1$, leading to a linear decrease in capillary pressure for $S_l < S_{lrc} + \varepsilon$, tangential to the standard Brooks-Corey curve at $S_l = S_{lrc} + \varepsilon$.

The curves shown in Figure 2.4.1.1 reflect the intended behavior, fulfilling Requirement 4.1.

**Figure 2.4.1.1.** Modified Brooks-Corey capillary pressure curves.

2.4.2 Modification to van Genuchten Capillary Pressure Function

The modified van Genuchten model is invoked by setting both IRP and ICP to 11. The model is described by the following set of equations (the input parameters are described in Table 2.4.2.1):

$$S_{ec} = \frac{S_l - S_{lrc}}{1 - S_{lrc}} \quad (2.4.2.1a)$$

$$S_{ek} = \frac{S_l - S_{lrk}}{1 - S_{lrk} - S_{gr}} \quad (2.4.2.1b)$$

$$p_c = -\frac{1}{\alpha} \left[(S_{ec})^{-1/m} - 1 \right]^{1/n} \quad \text{for } S_l \geq (S_{lrc} + \varepsilon) \quad (2.4.2.2a)$$

$$\text{linear model with continuous slope at } S_l = S_{lrc} + \varepsilon \quad \text{for } S_l < (S_{lrc} + \varepsilon) \quad (2.4.2.2b)$$

$$p_c \geq -p_{c,\max} \quad (2.4.2.3)$$

$$k_{rl} = S_{ek}^{1/2} \left[1 - (1 - S_{ek}^{1/m})^m \right]^2 \quad (2.4.2.4a)$$

$$k_{rg} = (1 - S_{ek})^{1/3} \left[1 - S_{ek}^{1/m} \right]^{2m} \quad (2.4.2.4b)$$

$$k_{rg} = 1 - k_{rl} \quad (2.4.2.4c)$$

Table 2.4.2.1. Input Parameters for Modified van Genuchten Model

Parameter	Variable	Description
IRP	11	select van Genuchten relative permeability model
$RP(1)$	S_{lrk}	residual liquid saturation for rel. perm. functions
$RP(2)$	S_{gr}	residual gas saturation
$RP(3)$	(flag)	if zero, use (2.4.2.4b), if non-zero, use (2.4.2.4c)
ICP	11	select van Genuchten capillary pressure model
$CP(1)$	n	analogous to pore size distribution index
$CP(2)$	$1/\alpha$	analogous to gas entry pressure [Pa]
$CP(3)$	ε or $p_{c,\max}$	if $CP(3) = 0$ then $p_{c,\max} = 10^{50}$, $\varepsilon = -1$ if $0 < CP(3) < 1$ use linear model (2.4.2.2b) for $S_l < S_{lr} + \varepsilon$ if $CP(3) \geq 1$, then $p_{c,\max} = CP(3)$, $\varepsilon = -1$
$CP(4)$	m	if zero then $m = 1 - 1/n$
$CP(6)$	S_{lrc}	if zero, then $S_{lrc} = S_{lrk}$

Figure 2.4.2.1 shows two modified van Genuchten capillary pressure functions. The first one, shown by the solid line, was produced with $CP(3) = p_{c,max} = 7000$, limiting the capillarity to values larger than $p_c = -7000$ Pa. The second curve, shown by the broken line, was produced with $CP(3) = \varepsilon = 0.1$, leading to a linear decrease in capillary pressure for $S_l < S_{lrc} + \varepsilon$, tangential to the standard van Genuchten curve at $S_l = S_{lrc} + \varepsilon$.

The curves shown in Figure 2.4.2.1 reflect the intended behavior, fulfilling Requirement 4.2.

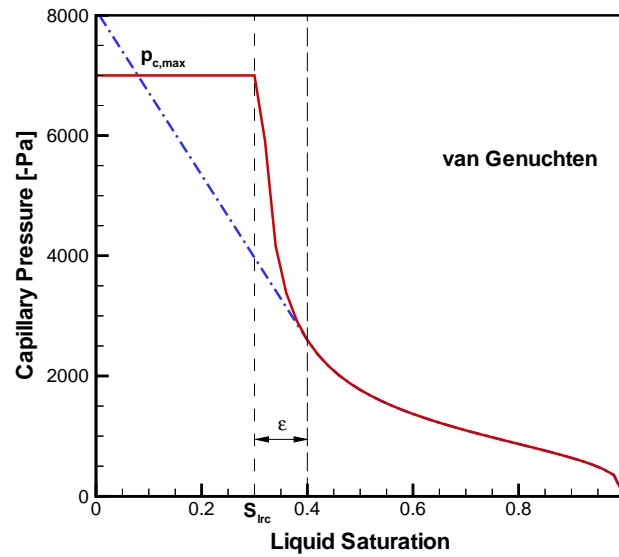


Figure 2.4.2.1. Modified van Genuchten capillary pressure curves.

2.5 New Observation Types

ITOUGH2 estimates TOUGH2 input parameters based on observations for which a corresponding TOUGH2 output variable is calculated. Two new observation types were added, i.e., new output variables are extracted from TOUGH2 and made available for comparison with observed data. In ITOUGH2, the observation type is specified by second-level commands in block `> OBSERVATION`. The first new observation type is selected by command `>> SECONDARY`, extracting the secondary parameters of the specified gridblock. The secondary parameters are the phase-specific fluid properties shown in Table 2.5.1 (see also Figure 2 in *Pruess [1991]*).

Table 2.5.1. Secondary Parameters

Index	Parameter
1	Saturation
2	Relative permeability
3	Dynamic viscosity
4	Density
5	Specific enthalpy
6	Capillary Pressure
NB+k	Mass fraction of Component k

The second new observation type is selected by command `>> HEAT FLOW`, extracting the heat flux of the specified connection.

The correct implementation of the new observation types is checked by comparing the values printed to the TOUGH2 output files with those reported as “computed” in the residual analysis of the ITOUGH2 output file. If they are identical, ITOUGH2 correctly extracted the selected values from the TOUGH2 output arrays.

File *vvi* shown in Figure 2.5.1 was used in combination with the TOUGH2 input file *vv* (see Figure 2.3.1) to generate the requested output. Note that `MOP(5)` is set to 8 in file *vv* to produce printout of all secondary parameters.

The following command was used:

```
itough2 -v 3.2 vvi vv 3 &
```

The output of this run is also used for testing Requirement 6.

```

> PARAMETERS

--- the following block tests new handling of porosity values,
    i.e., porosity given in block INCON (0.5) will be overwritten by
    initial guess (0.6) for elements with rock type BC___ (ELM 2)

>> POROSITY
  >>> MATERIAL: BC___
    >>>> VALUE
    >>>> GUESS: 0.6
    <<<<
  <<<
<<

> OBSERVATION

>> TIME: 1
    1.0

--- The following blocks test the new observation type SECONDARY

>> SECONDARY parameters

--- gas phase

  >>> ELEMENT: ELM_1
    >>>> ANNOTATION: 1,1=gas sat
    >>>> GAS PHASE
    >>>> PARAMETER : 1
    >>>> NO DATA
    <<<<
  >>> ELEMENT: ELM_1
    >>>> ANNOTATION: 1,2=gas rel per
    >>>> GAS PHASE
    >>>> PARAMETER : 2
    >>>> NO DATA
    <<<<
  >>> ELEMENT: ELM_1
    >>>> ANNOTATION: 1,3=gas visc
    >>>> GAS PHASE
    >>>> PARAMETER : 3
    >>>> NO DATA
    <<<<
  >>> ELEMENT: ELM_1
    >>>> ANNOTATION: 1,4=gas dens
    >>>> GAS PHASE
    >>>> PARAMETER : 4
    >>>> NO DATA
    <<<<

```

Figure 2.5.1. ITOUGH2 input file *vvi*.

```

>>> ELEMENT: ELM_1
>>>> ANNOTATION: 1,5=gas enth
>>>> GAS PHASE
>>>> PARAMETER : 5
>>>> NO DATA
<<<<
>>> ELEMENT: ELM_1
>>>> ANNOTATION: 1,6=gas cap pres
>>>> GAS PHASE
>>>> PARAMETER : 6
>>>> NO DATA
<<<<
>>> ELEMENT: ELM_1
>>>> ANNOTATION: 1,7=Xwg
>>>> GAS PHASE
>>>> PARAMETER : 7
>>>> NO DATA
<<<<
>>> ELEMENT: ELM_1
>>>> ANNOTATION: 1,8=Xag
>>>> GAS PHASE
>>>> PARAMETER : 8
>>>> NO DATA
<<<<

--- liquid phase

>>> ELEMENT: ELM_1
>>>> ANNOTATION: 2,1=liq sat
>>>> LIQUID PHASE
>>>> PARAMETER : 1
>>>> NO DATA
<<<<
>>> ELEMENT: ELM_1
>>>> ANNOTATION: 2,2=liq rel per
>>>> LIQUID PHASE
>>>> PARAMETER : 2
>>>> NO DATA
<<<<
>>> ELEMENT: ELM_1
>>>> ANNOTATION: 2,3=liq visc
>>>> LIQUID PHASE
>>>> PARAMETER : 3
>>>> NO DATA
<<<<
>>> ELEMENT: ELM_1
>>>> ANNOTATION: 2,4=liq dens
>>>> LIQUID PHASE
>>>> PARAMETER : 4
>>>> NO DATA
<<<<

```

Figure 2.5.1. (cont.) ITOUGH2 input file *vvi*.

```

>>> ELEMENT: ELM_1
>>>> ANNOTATION: 2,5=liq enth
>>>> LIQUID PHASE
>>>> PARAMETER : 5
>>>> NO DATA
<<<<
>>> ELEMENT: ELM_1
>>>> ANNOTATION: 2,6=liq cap pres
>>>> LIQUID PHASE
>>>> PARAMETER : 6
>>>> NO DATA
<<<<
>>> ELEMENT: ELM_1
>>>> ANNOTATION: 2,7=Xw1
>>>> LIQUID PHASE
>>>> PARAMETER : 7
>>>> NO DATA
<<<<
>>> ELEMENT: ELM_1
>>>> ANNOTATION: 2,8=Xa1
>>>> LIQUID PHASE
>>>> PARAMETER : 8
>>>> NO DATA
<<<<
<<<

--- the following block tests new observation type HEAT FLOW

>> HEAT FLOW
>>> CONNECTION:  ELM_1 ELM_2
>>>> NO DATA
<<<<
<<<
<<

> COMPUTATION
>> OUTPUT
>>> VERSION control statements
>>> CHARACTERISTIC curves
<<<

>> OPTION
>>> FORWARD
<<<
<<
<

```

Figure 2.5.1. (cont.) ITOUGH2 input file *vvi*.

Figure 2.5.2 shows an excerpt from the TOUGH2 output file. As a result of option MOP(5)=8, the secondary parameters as stored in TOUGH2 vector PAR are printed for gridblock “ELM 1”, providing information about viscosity, specific enthalpy, and water mass fractions not available in the standard TOUGH2 output file. Saturation, relative permeability, capillary pressure, air mass fractions, and phase densities can be taken from the standard TOUGH2 output. Heat flow across interface “ELM 2 ELM 1” is -353.11 W.

Figure 2.5.3 shows an excerpt from the ITOUGH2 output file *vvi.out*. The column under header “COMPUTED” holds the selected observations extracted from TOUGH2 vector PAR and GLO for the specified gridblock and connection, respectively.

The values given in column “COMPUTED” of file *vvi.out* (Figure 2.5.3) and the corresponding output variables in the TOUGH2 output file (Figure 2.5.2) are identical, confirming the correct implementation of Requirement 5.


```

=====
RESIDUAL ANALYSIS
=====
RESIDUAL : Measured - computed
R*P*R    : Squared weighted residual
STD. DEV.: A posteriori standard deviation of computed system response
Yi       : Local reliability or influence. Observations with Yi < 0.25 are poorly controlled.
Wi       : Normalized residual. If abs(Wi) > u(0.99) = 2.58 observation is potential outlier.
=====

```

#	OBSERVATION	AT TIME [sec]	MEASURED	COMPUTED	RESIDUAL	WEIGHT	R*P*R	STD. DEV.	Yi	Wi
1	POROSITY BC		0.20000E+00	0.60000E+00	-0.40000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
2	1,1=gas sat	0.10000E+01	0.10000E-49	0.30002E+00	-0.30002E+00	0.10000E+01	0.90014E-01	0.00000E+00	1.00	-0.30
3	1,2=gas rel per	0.10000E+01	0.10000E-49	0.86822E+00	-0.86822E+00	0.10000E+01	0.75381E+00	0.00000E+00	1.00	-0.87
4	1,3=gas visc	0.10000E+01	0.10000E-49	0.19069E-04	-0.19069E-04	0.10000E+01	0.36363E-09	0.00000E+00	1.00	0.00
5	1,4=gas dens	0.10000E+01	0.10000E-49	0.11114E+01	-0.11114E+01	0.10000E+01	0.12353E+01	0.00000E+00	1.00	-1.11
6	1,5=gas enth	0.10000E+01	0.10000E-49	0.31337E+06	-0.31337E+06	0.10000E+01	0.98203E+11	0.00000E+00	1.00	***** *
7	1,6=gas cap pre	0.10000E+01	0.10000E-49	0.00000E+00	0.10000E-49	0.10000E+01	0.10000E-99	0.00000E+00	1.00	0.00
8	1,7=Xwg	0.10000E+01	0.10000E-49	0.74692E-01	-0.74692E-01	0.10000E+01	0.55789E-02	0.00000E+00	1.00	-0.07
9	1,8=Xag	0.10000E+01	0.10000E-49	0.92531E+00	-0.92531E+00	0.10000E+01	0.85620E+00	0.00000E+00	1.00	-0.93
10	2,1=liq sat	0.10000E+01	0.10000E-49	0.69998E+00	-0.69998E+00	0.10000E+01	0.48997E+00	0.00000E+00	1.00	-0.70
11	2,2=liq rel per	0.10000E+01	0.10000E-49	0.13178E+00	-0.13178E+00	0.10000E+01	0.17365E-01	0.00000E+00	1.00	-0.13
12	2,3=liq visc	0.10000E+01	0.10000E-49	0.54417E-03	-0.54417E-03	0.10000E+01	0.29613E-06	0.00000E+00	1.00	0.00
13	2,4=liq dens	0.10000E+01	0.10000E-49	0.98807E+03	-0.98807E+03	0.10000E+01	0.97629E+06	0.00000E+00	1.00	-988.07 *
14	2,5=liq enth	0.10000E+01	0.10000E-49	0.20934E+06	-0.20934E+06	0.10000E+01	0.43821E+11	0.00000E+00	1.00	***** *
15	2,6=liq cap pre	0.10000E+01	0.10000E-49	-0.70715E+03	0.70715E+03	0.10000E+01	0.50006E+06	0.00000E+00	1.00	707.15 *
16	2,7=Xwl	0.10000E+01	0.10000E-49	0.99998E+00	-0.99998E+00	0.10000E+01	0.99997E+00	0.00000E+00	1.00	-1.00
17	2,8=Xal	0.10000E+01	0.10000E-49	0.15337E-04	-0.15337E-04	0.10000E+01	0.23524E-09	0.00000E+00	1.00	0.00
18	F-H ELM 1 ELM 2	0.10000E+01	0.10000E-49	-0.35311E+03	0.35311E+03	0.10000E+01	0.12469E+06	0.00000E+00	1.00	353.11 *

Figure 2.5.3. Excerpt from ITOUGH2 output file *vvi.out*, showing residual analysis.

2.6 New Priorities in Assigning Porosities

In standard TOUGH2, porosity is specified through variable POR in block ROCKS. This value is assigned to all gridblocks which belong to the corresponding rock type. However, this porosity value can be overwritten on a gridblock-to-gridblock basis through variable PORX specified in block INCON. If porosity is one of the parameters to be estimated by inverse modeling, the porosity should be adjusted during the optimization, i.e., the porosity estimate provided by ITOUGH2 must have the highest priority, overwriting values stored in POR and PORX.

In order to test the implementation of this concept, we used three different ways to assign porosity to gridblocks “ELM 1”, “ELM 2”, and “ELM 3” as shown in file *vv* (Figure 2.3.1) and *vv1* (Figure 2.5.1). The initial guess for porosity specified in the ITOUGH2 input file is different from the corresponding one in the TOUGH2 input file, affecting “ELM 2”. Porosity values are also given in block INCON for gridblocks “ELM 1” and “ELM 2”. The porosities given in SAVE file *vv.sav* (Figure 2.6.1) reflect the values actually used in the simulation.

A summary is given in Table 2.6.1. The porosity value from block INCON has overwritten that from block ROCKS, and the porosity given in the ITOUGH2 input file has overwritten that from block INCON, in agreement with the intended behavior and thus fulfilling Requirement 6.

```

INCON -- INITIAL CONDITIONS FOR      3 ELEMENTS AT TIME  0.100000E+01
ELM 1          0.40000000E+00
  0.1077494458364E+06  0.1030002349086E+02  0.4999944736214E+02
ELM 2          0.60000000E+00
  0.1013411139066E+06  0.1029998794249E+02  0.2000110000267E+02
ELM 3          0.30000000E+00
  0.1000491003565E+06  0.1029999300758E+02  0.2000000330247E+02
+++
  1    3    5  0.00000000E+00  0.10000000E+01

```

Figure 2.6.1. File *vv.sav* showing porosity values used during the simulation.

Table 2.6.1. Porosities Assigned and Actually Used

Gridblock	ROCKS	INCON	ITOUGH2	SAVE
ELM 1	0.1	0.4	-	0.4
ELM 2	0.2	0.5	0.6	0.6
ELM 3	0.3	-	-	0.3

2.7 Adjusting Array Dimensions

Problems solved by ITOUGH2 vary considerably in size, depending on the number of gridblocks and connections used for discretization, the number of equations solved, the number of parameters estimated, the number of observations available, etc. Due to the overall size of ITOUGH2, it is important to be able to adjust the dimensions of major TOUGH2 and ITOUGH2 arrays to make the code fit on a specific computer with limited memory. Because ITOUGH2 is written in FORTRAN77, no dynamic memory allocation is possible, i.e., arrays are redimensioned by changing their size in the source code, followed by recompilation.

The design and architecture of ITOUGH2 allows for safe, convenient, and fast adjustment of major arrays. The purpose of this section is to prove that changing array dimensions using the procedure described herein does not corrupt the code.

The ITOUGH2 design makes use of the following features to assure safe maintenance of the code:

- (1) All COMMON blocks holding major arrays are stored in INCLUDE files, making sure that any modification (such as redimensioning) is made consistently throughout the code.
- (2) Array dimensions are given by constants, which are defined using PARAMETER statements. This assures consistency of arrays that must have identical dimensions. The PARAMETER statements are summarized in an INCLUDE file named *maxsize.inc*.
- (3) Compilation is performed by means of a makefile and the “make” utility, available on UNIX machines and most PCs. This assures that all files affected by a change are recompiled.
- (4) Checks are made within ITOUGH2 to assure that a given array is sufficiently large to accommodate the problem at hand. If an array index is greater than the size of the array, an error message is printed and ITOUGH2 run is stopped.
- (5) The array dimensions used for a specific run are reported in output files for traceability (see Section 2.8).

The procedure for redimensioning major arrays can be described as follows:

- (1) If an ITOUGH2 array is not sufficiently dimensioned, an error message is issued, indicating the constant that must be increased.
- (2) The user edits file *maxsize.inc*, adjusting the appropriate constants.
- (3) The user types “make” to recompile and relink ITOUGH2.

The following test runs assure that (A) ITOUGH2 cannot be run if an array is insufficiently dimensioned, and (B) if ITOUGH2 runs, its arrays are sufficiently dimensioned.

In order to perform Test A, the constants defined in file *maxsize.inc* were stepwise reduced until an error message was issued when running the recompiled code using the following command:

```
itough2 -v 3.2 vvRITi vvRIT 3 &
```

An example of an error message is shown in Figure 2.7.1.

The constants were then increased by 1 above the values that triggered the error message, yielding the minimum array sizes accepted by ITOUGH2. The corresponding file (named *minsize.inc*) is shown in Figure 2.7.2.

ITOUGH2 was then recompiled using minimum array dimensions, and a compiler option, which detects array size violations during compilation and execution. The on-line manual pages for the corresponding compiler option for the SUN Solaris 2 compiler f77, Version FORTRAN 77, SC4.2, are reproduced in Figure 2.7.3.

Adjusting array dimensions can be considered safe if ITOUGH2 compiles and runs properly with array dimensioned minimally for the given test problem, since array range violations are most rigorously detected with minimum array dimensions. If arrays are larger than the problem size, no problems are expected to occur. If array dimensions are too large to make ITOUGH2 fit in the computer's memory, either the code cannot be run, or its speed performance deteriorates. Neither case poses a risk that erroneous simulation results are obtained.

ITOUGH2 could be compiled and run with minimum array dimensions, fulfilling Requirement 7.

```
***** ERROR *****
* Number of parameters exceeds MAXN = 2.
* Increase MAXN in file maxsize.inc and recompile!
***** ERROR *****
```

Figure 2.7.1. Excerpt from ITOUGH2 output file *vvRITi.out*, show error message if arrays are insufficiently dimensioned.

```

C$$$$$$$$$ PARAMETERS FOR SPECIFYING THE MAXIMUM PROBLEM SIZE $$$$$$$$$$
C
C *****
C ITOUGH2 and TOUGH2 parameter statements
C *****
C
C --- MAXTIM   : Maximum number of calibration times
C               INTEGER MAXTIM
C               PARAMETER (MAXTIM=61)
C
C *****
C TOUGH2 parameter statements
C *****
C
C --- MAXEL    : Maximum number of elements
C               INTEGER MAXEL
C               PARAMETER (MAXEL=53)
C
C --- MAXCON   : Maximum number of connections
C               INTEGER MAXCON
C               PARAMETER (MAXCON=52)
C
C --- MAXK     : Maximum number of components/species
C               INTEGER MAXK
C               PARAMETER (MAXK=2)
C
C --- MAXEQ    : Maximum number of equations per block
C               INTEGER MAXEQ
C               PARAMETER (MAXEQ=3)
C
C --- MAXPH    : Maximum number of phases
C               INTEGER MAXPH
C               PARAMETER (MAXPH=2)
C
C --- MAXB     : Maximum number of phase-dependent secondary variables
C               other than component mass fractions
C               INTEGER MAXB
C               PARAMETER (MAXB=6)
C
C --- MAXSS    : Maximum number of sources/sinks
C               INTEGER MAXSS
C               PARAMETER (MAXSS=1)
C
C --- MAVTAB   : Maximum average number of table entries per sink/source
C               INTEGER MAVTAB
C               PARAMETER (MAVTAB=1)
C
C --- MAXROC   : Maximum number of rock types
C               INTEGER MAXROC
C               PARAMETER (MAXROC=3)
C
C --- MAXTSP   : Maximum number of specified time steps divided by 8
C               INTEGER MAXTSP
C               PARAMETER (MAXTSP=1)
C
C --- MAXLAY   : Maximum number of reservoir layers for deliverability
C               INTEGER MAXLAY
C               PARAMETER (MAXLAY=1)
C
C --- MAXRPCP  : Maximum number of parameters for a relative permeability
C               or a capillary pressure function
C               (to get more than 7, more input lines may be needed!).
C               INTEGER MXRPCP
C               PARAMETER (MXRPCP=7)
C
C --- MXPCTB   : Maximum points in table of ECM capillary pressure
C               vs. saturation
C               INTEGER MXPCTB
C               PARAMETER (MXPCTB=1)
C
C --- MXTBC    : Maximum number of elements with time vs. boundary condition
C --- MXTBPT   : Maximum number of time vs. pressure data
C               INTEGER MXTBC,MXTBPT
C               PARAMETER (MXTBC=1)
C               PARAMETER (MXTBPT=1)

```

Figure 2.7.2. File *maxsize.inc* with minimum array dimensions for test problem.

```

C --- Storage for MA28. LIRN is the size of IRN and needs to be larger
C than the number of non-zeros NZ=(NEL+2*NCON)*NEQ*NEQ.
C LICN is the length of ICN and CO.
C   INTEGER LICN,LIRN
C   PARAMETER (LIRN=2*(MAXEL+2*MAXCON)*MAXEQ*MAXEQ)
C   PARAMETER (LICN=4*(MAXEL+2*MAXCON)*MAXEQ*MAXEQ)
C
C --- Parameters for conjugate gradient package t2cg1
C   INTEGER NREDM,MNZ,NRWORK,NIWORK
C   PARAMETER (NREDM=MAXEQ*MAXEL)
C   PARAMETER (MNZ=(MAXEL+2*MAXCON)*MAXEQ*MAXEQ)
C   PARAMETER (NRWORK=1000+MNZ+38*NREDM)
C   PARAMETER (NIWORK=32+MNZ+5*NREDM)
C
C --- Parameters for IFS
C   MAXIFSP : Maximum number of IFS parameters
C   INTEGER MAXIFSP
C   PARAMETER (MAXIFSP=1)
C
C *****
C ITOUGH2 parameter statements
C *****
C --- MAXN : Maximum number of parameters to be estimated
C   INTEGER MAXN
C   PARAMETER (MAXN=3)
C
C --- MAXO : Maximum number of datasets
C   INTEGER MAXO,MAXOTWO
C   PARAMETER (MAXO=2)
C   PARAMETER (MAXOTWO=2*MAXO)
C
C --- MAXM : Maximum number of calibration points
C (approx. number of datasets times number of calibration times)
C   INTEGER MAXM
C   PARAMETER (MAXM=123)
C
C --- MAXPD : Max number of paired data
C   INTEGER MAXPD
C   PARAMETER (MAXPD=120)
C
C --- MAXR : Dimension of array RPAR and IPAR, ROBS and IOBS
C   INTEGER MAXR
C   PARAMETER (MAXR=10)
C
C --- MAXBRK : Max number of points in time at which SAVE file is written (restart)
C   INTEGER MAXBRK
C   PARAMETER (MAXBRK=1)
C
C --- MAXEBRK : Max number of elements with new initial conditions after break
C   INTEGER MAXEBRK
C   PARAMETER (MAXEBRK=1)
C
C --- MAXCOEFF : Max number of coefficients for data modeling functions
C   INTEGER MAXCOEFF
C   PARAMETER (MAXCOEFF=1)
C
C --- MAXMCS : Max number of Monte Carlo simulations
C   INTEGER MAXMCS
C   PARAMETER (MAXMCS=1)
C
C --- MAXCURVE : Max number of curves to be plotted
C   INTEGER MAXCURVE
C   PARAMETER (MAXCURVE=6)

```

Figure 2.7.2. (cont.) File *maxsize.inc* with minimum array dimensions for test problem.


```
F77(1)                User Commands                F77(1)

NAME
    f77 - FORTRAN 77 compiler
...

DESCRIPTION
    f77 is a superset of FORTRAN 77.
    Version:  FORTRAN 77 SC4.2
...

-C    Check array references for out of range subscripts.

      Subscripting arrays beyond their declared sizes may
      result in unexpected results, including segmentation
      faults. The -C option checks for possible array sub-
      script violations in the source code and during execu-
      tion.

      If the -C option is used, array subscript violations
      are treated as an error. If an array subscript range
      violation is detected in the source code during compi-
      lation, it is treated as a compilation error.

      This option will increase the size of the executable
      file.
```

Figure 2.7.3. Manual pages for compiler option `-C`, checking array subscript violations.

2.8 Application Control

The application control of ITOUGH2 simulations was enhanced to improve traceability. The following information is printed to either the TOUGH2 output file, the ITOUGH2 output file, or the ITOUGH2 message file:

- Starting and ending date and time of run;
- Names of TOUGH2 and ITOUGH2 input files;
- Directory name of input and output files;
- Equation-of-state module used;
- Name of script file used to run ITOUGH2;
- Command arguments passed to script file;
- Name of ITOUGH2 executable;
- Type of computer used;
- Computer host name;
- Login name of user;
- Constants used for dimensioning of major arrays (see Section 2.7);
- Version control statements for each subroutine.

Figures 2.8.1 through 2.8.4 show various excerpts of the ITOUGH2 output file *vvRITi.out*. Note the correct reporting of command line arguments, and the array dimension statements, which agree with the values given in include file *maxsize.inc*, shown in Figure 2.7.2. Requirement 8 is considered fulfilled.


```

=====
      ARRAY DIMENSIONS (SEE FILE maxsize.inc)
-----
MAXEL      =      53      Maximum number of elements
MAXCON     =      52      Maximum number of connections
MAXK       =          2      Maximum number of components
MAXEQ      =          3      Maximum number of equations
MAXPH      =          2      Maximum number of phases
MAXB       =          6      Maximum number of phase-dependent secondary variables
MAXSS      =          1      Maximum number of sinks/sources
MAVTAB     =          1      Maximum average number of table entries per sink/source
MAXROC     =          3      Maximum number of rock types
MAXTSP     =          1      Maximum number of specified time steps, divided by eight
MAXLAY     =          1      Maximum number of reservoir layers for wells on deliverability
MXRPCP     =          7      Maximum number of parameters for relative permeability and capillary pressure functions
MXPCTB     =          1      Maximum number of points in table for ECM capillary pressure
MXTBC      =          1      Maximum number of elements with time vs. boundary condition
MXTBCT     =          1      Maximum number of time vs. pressure data
MAXTIM     =         61      Maximum number of calibration times
MAXN       =          3      Maximum number of parameters to be estimated
MAXO       =          2      Maximum number of datasets
MAXM       =        123      Maximum number of calibration points
MAXPD      =        120      Maximum number of paired data
MAXR       =         10      Maximum number of elements or indices of each parameter or observation
MAXBRK     =          1      Maximum number of points in time at which SAVE file is written for restart
MAXEBRK    =          1      Maximum number of elements with new initial conditions after restart
MAXCOEFF   =          1      Maximum number of coefficients for data modeling functions
MAXMCS     =          1      Maximum number of Monte Carlo simulations
MAXCURVE   =          6      Maximum number of curves to be plotted
MAXXGR     =          3      Dimension of third index of array XGUESSR
MTYPE      =         17      Number of observation types
MPFMT      =          6      Number of plot file formats
MAXPV      =          4      Maximum number of primary variables
-----

```

Figure 2.8.3. Excerpt from ITOUGH2 output file *vvRITi.out*, showing information regarding computer system used and command line arguments.

PROGRAM	VERSION	DATE	COMMENT
ITOUGH2		Current version	V3.2 (May 1998)
ITOUGH	1.0	1 AUGUST 1992	ITOUGH User's Guide, Version 1.0, Report NIB 92-99
ITOUGH2	2.2	1 FEBRUARY 1994	ITOUGH2 User's Guide, Version 2.2, Report LBL-34581
ITOUGH2	3.0	12 JULY 1996	YMP Software qualification, Report LBNL-39489
ITOUGH2	3.1	1 APRIL 1997	ITOUGH2 Command Reference, Version 3.1, Report LBNL-40041
ITOUGH2	3.2	1 JULY 1998	YMP Software qualification, Report LBNL-42002
WHATCOM	1.0	10 AUGUST 1993	#35: Q: WHAT COMPUTER IS USED? A: SUN
CALLSIG	1.0	5 DECEMBER 1995	#112: SIGNAL HANDLER
CPUSEC	1.0	10 AUGUST 1993	#--: RETURNS CPU-TIME (VERSION SUN)
OPENFILE	2.5	4 JUNE 1996	#31: OPENS MOST OF THE FILES
LENOS	1.0	1 MARCH 1992	#28: RETURNS LENGTH OF LINE
PREC	1.0	1 AUGUST 1992	#86: CALCULATE MACHINE DEPENDENT CONSTANTS
ITHEADER	3.2	27 MAY 1998	#29: PRINTS ITOUGH2 HEADER
DAYTIM	1.0	10 AUGUST 1993	#32: RETURNS DATE AND TIME (VERSION SUN)
THEADER	3.2	27 MAY 1998	#30: PRINTS TOUGH2 HEADER
INPUT	3.2	20 JUNE 1998	READ ALL DATA PROVIDED THROUGH FILE *INPUT*, + SECONDARY MESH + USERX
CHECKMAX	1.0	11 MAY 1996	#41: CHECK KEY DIMENSIONS
FLOPP	1.0	11 APRIL 1991	CALCULATE NUMBER OF SIGNIFICANT DIGITS FOR FLOATING POINT ARITHMETIC
RFILE	3.2	21 OCTOBER 1997	INITIALIZE DATA FROM FILES *MESH* OR *MINC*, *GENER*, AND *INCON*
ITINPUT	1.0	1 AUGUST 1992	# 2: READS COMMANDS OF COMMAND LEVEL 1
READCOMM	2.5	14 JUNE 1996	#24: READS A COMMAND
FINDKEY	1.1	4 AUGUST 1993	#25: READS A KEYWORD
LTU	1.0	1 AUGUST 1992	#26: CONVERTS LOWER TO UPPER CASE
INPARAM	3.2	20 JUNE 1998	# 3: READS PARAMETERS TO BE ESTIMATED
INPAR	3.1	17 MARCH 1997	# 4: READS PARAMETER VALUES, WEIGHTS, ETC.
INELEM	3.1	3 APRIL 1997	#23: READS GRID BLOCK NAME AFTER A COLON
NEXTWORD	2.5	9 FEBRUARY 1996	#27: EXTRACTS NEXT WORD ON A LINE
INWBP	3.1	17 MARCH 1997	#11: READS WEIGHT, BOUNDS, ANNOTATION, AND PARAMETERS
READREAL	1.0	1 AUGUST 1992	#22: READS A REAL AFTER A COLON
READINT	1.0	1 AUGUST 1992	#21: READS AN INTEGER AFTER A COLON
INOBSERV	3.2	2 OCTOBER 1997	#12: READS TYPE OF OBSERVATION
INTIMES	3.1	29 APRIL 1997	#13: READS TIMES AT WHICH OBSERVATIONS ARE AVAILABLE
INOBS	2.5	13 DECEMBER 1995	#15: READS OBSERVATION INFOS
INOBSDAT	2.5	13 JANUARY 1996	#17: READS ALL OBSERVED DATA
INPAIRED	3.1	2 APRIL 1997	#19: READS PAIRED DATA SET
INWEIGHT	3.2	7 OCTOBER 1997	#20: READS WEIGHTS
INCOMPUT	1.0	1 AUGUST 1992	#16: READS VARIOUS COMPUTATIONAL PARAMETERS
INTOLER	3.1	27 MARCH 1997	#83: READS TOLERANCE/STOPPING CRITERIA
INERROR	2.3	20 DECEMBER 1994	#81: READS COMMANDS FOR ERROR ANALYSIS
INPRINT	2.5	13 JANUARY 1996	#80: READS OUTPUT OPTIONS
GETINDEX	2.2	11 MARCH 1994	#45: GETS INDEX OF ELEMENTS, CONNECTIONS, AND SOURCES
INIGUESS	3.2	20 JUNE 1998	#38: INITIAL GUESS OF PARAMETERS (XGUESS)

Figure 2.8.4. Excerpt from ITOUGH2 output file *vvRITi.out*, showing version control statements.

GETNMAT	2.1	21	SEPTEMBER	1993	#44: IDENTIFIES MATERIAL NUMBER
IXLBXUB	2.1	21	SEPTEMBER	1993	#43: INITIALIZES ARRAY XLB AND XUB
SETWSCAL	2.5	8	AUGUST	1996	#39: INITIALIZES ARRAY WSCALE
OBSMEAN	1.0	1	AUGUST	1992	#40: CALCULATES MEAN OF OBSERVATIONS
SETXSCAL	1.0	1	AUGUST	1992	#42: INITIALIZES ARRAY XSCALE
IN_OUT	3.2	20	JUNE	1998	#35: PRINTS A SUMMARY OF INPUT DATA
TIMEWIND	2.5	30	NOVEMBER	1995	#53: SETS TIME WINDOW
PRSTATUS	3.1	20	FEBRUARY	1997	#91: PRINTS STATUS MESSAGES
ERRORMSG	2.5	21	MARCH	1996	#34: PRINTS ERROR MESSAGES
LEVVAR	2.5	26	MARCH	1996	#99: LEVENBERG-MARQUARDT OPTIMIZATION ALGORITHM
FCNLEV	2.3	10	JANUARY	1995	#50: RETURNS WEIGHTED RESIDUAL VECTOR
UPDATE	3.2	20	JUNE	1998	#37: UPDATES PARAMETERS
PRIORINF	2.1	21	SEPTEMBER	1993	#48: PRIOR INFORMATION
OBSERVAT	3.2	2	OCTOBER	1997	#62: COMPARES MEASURED AND CALCULATED QUANTITIES
GETMESH	1.1	15	APRIL	1993	#47: READS FILE MESH, MINC, GENER, AND INCON
GETINCON	3.2	18	NOVEMBER	1997	#46: READS FILE INCON
INITTOUG	2.5	18	APRIL	1996	#54: INITIALIZES TOUGH2 RUN (REPLACES CYCIT)
EOS	1.0	28	MARCH	1991	*EOS3* ... THERMOPHYSICAL PROPERTIES MODULE FOR WATER/AIR
SAT	1.0	22	JANUARY	1990	STEAM TABLE EQUATION: SATURATION PRESSURE AS FUNCTION OF TEMPERATURE
VISW	1.0	22	JANUARY	1990	VISCOSITY OF LIQUID WATER AS FUNCTION OF TEMPERATURE AND PRESSURE
COWAT	1.0	22	JANUARY	1990	LIQUID WATER DENSITY AND INT. ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE
PCAP	3.2	1	JUNE	1998	CAPILLARY PRESSURE
SUPST	1.0	29	JANUARY	1990	VAPOR DENSITY AND INTERNAL ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE
VISCO	1.0	1	FEBRUARY	1990	CALCULATE VISCOSITY OF VAPOR-AIR MIXTURES
COVIS	1.0	1	FEBRUARY	1990	COEFFICIENT FOR GAS PHASE VISCOSITY CALCULATION
VISS	1.0	22	JANUARY	1990	VISCOSITY OF VAPOR AS FUNCTION OF TEMPERATURE
RELPER	3.2	1	JUNE	1998	RELATIVE PERMEABILITIES
BALLA	1.0	5	MARCH	1991	PERFORM SUMMARY BALANCES FOR VOLUME, MASS, AND ENERGY
INDATA	1.0	5	MARCH	1991	PROVIDE PRINTOUT OF MOST DATA PROVIDED THROUGH FILE *INPUT*
CALLTOUG	3.1	2	APRIL	1997	#55: CALLS TOUGH2 FOR ONE TIME STEP
TSTEP	3.1	27	MARCH	1997	ADJUST TIME STEPS TO COINCIDE WITH USER-DEFINED TARGET TIMES
MULTI	3.2	1	JUNE	1998	ASSEMBLE ALL ACCUMULATION AND FLOW TERMS
LINEQ	0.91 CG	31	JANUARY	1994	INTERFACE FOR LINEAR EQUATION SOLVERS
CONVER	2.5	13	JUNE	1996	CAN CALL MA28 OR A PACKAGE OF CONJUGATE GRADIENT SOLVERS
OUT	2.5	18	APRIL	1996	UPDATE PRIMARY VARIABLES AFTER CONVERGENCE IS ACHIEVED
OBSERVED	2.4	4	AUGUST	1996	PRINT RESULTS FOR ELEMENTS, CONNECTIONS, AND SINKS/SOURCES
OBJFUN	2.5	21	MARCH	1996	#78: RETURNS OBSERVED DATA AS A FUNCTION OF TIME
WRITEPAR	1.0	17	JUNE	1996	#49: COMPUTE OBJECTIVE FUNCTION
PLOTFILE	3.2	6	OCTOBER	1997	#56: WRITE BEST FIT PARAMETER SET AND BLOCK ROCKS
JAC	3.1	24	FEBRUARY	1997	#58: WRITES PLOTFILE IN PLOPO-FORMAT
MLLAMBDA	2.2	14	FEBRUARY	1994	#51: CALCULATES FINITE DIFFERENCE JACOBIAN
TERMINAT	3.2	13	MAY	1998	#67: ESTIMATES NEW LAMBDA
WRIFI	2.5	13	JANUARY	1996	61: PERFORM ERROR ANALYSIS AND TERMINATE ITOUGH2
QFISHER	2.2	16	FEBRUARY	1994	AT THE COMPLETION OF A TOUGH2 RUN, WRITE PRIMARY VARIABLES ON FILE *SAVE*
QCHI	1.0	1	AUGUST	1992	#77: RETURNS QUANTILE OF F-DISTRIBUTION
POLYNOM	1.0	1	AUGUST	1992	#88: RETURNS CHI-SQUARE QUANTILE
					#89: EVALUATES POLYNOM

Figure 2.8.4. (cont.) Excerpt from ITOUGH2 output file *vvRITi.out*, showing version control statements.

```
EIGEN      3.2      14 AUGUST   1997      #59: PERFORMS EIGENANALYSIS
LOGLIKE    2.1      29 SEPTEMBER 1993      #68: COMPUTE LOG-LIKELIHOOD
QNORMAL    2.5      13 JANUARY   1996      #87: RETURNS QUANTILE OF NORMAL DISTRIBUTION
MOMENT     3.2      23 JULY      1997      #90: MOMENTS OF DISTRIBUTION
SORT       3.1      17 APRIL     1997      #113: SORTS ARRAY
MOMENT     3.1      17 APRIL     1997      #75: LINEAR REGRESSION ANALYSIS
PLOTIF     1.0      15 FEBRUARY  1993      #96: PLOT INTERFACE
REFORMAT   1.1      15 APRIL     1993      #97: REFORMATS PLOT FILES
QUOTES     1.0      15 FEBRUARY  1993      #98: RETURNS TEXT BETWEEN QUOTES

=====
---      2nd ITOUGH2 simulation job completed: 25-Jun-98  10:51 --- CPU time used =      77.82 sec.
---      0 error(s) and  0 warning(s) detected
```

Figure 2.8.4. (cont.) Excerpt from ITOUGH2 output file *vvRITi.out*, showing version control statements.

2.9 Regression Testing

The purpose of regression testing is to make sure that the various modifications made to ITOUGH2 have not corrupted the overall performance of the code. An inversion is performed in the following test case, i.e., the main application model of ITOUGH2 is tested, engaging almost all subroutines and major program options. However, the test case does not make use of any of the new features presented in this report, which makes it compatible with the previously qualified version of the code (ITOUGH2 V3.0, *Finsterle et al.* [1996]).

The same test case is run with Versions 3.0 and 3.2, using the following two commands:

```
itough2 -v 3.0 -ito vvRITi.v30.out vvRITi vvRIT 3 &  
itough2 -v 3.2 vvRITi vvRIT 3 &
```

The test case is similar to sample problem *sam1p4i*, described in detail in *Finsterle* [1997]. A comparison of output file *vvRITiv30.out* (Figure 2.9.1) with file *vvRITi.out* (Figure 2.9.2) shows that identical parameter estimates and estimation uncertainties were obtained, passing the regression test and fulfilling Requirement 9.

It is suggested to use this test case also for installation testing when porting ITOUGH2 from one platform to another.

3. Summary

Table 3.1 summarizes the test cases run to qualify ITOUGH2 V3.2 by listing the requirements (see also SCMS Form 2, Point 4), the associated input and relevant output files, and the outcome of the test, i.e., whether the acceptance criteria (SCMS Form 3, Point 1) were met.

Table 3.1. Summary of V & V Testing

#	Requirement	Input Files	Output Files	Criteria Met?
	Fracture-matrix interface area reduced by:			
1.1	A constant	<i>vvFM1A</i> <i>vvFM1B</i>	<i>vvFM1A.out</i> <i>vvFM1B.out</i>	yes
1.2	Upstream saturation	<i>vvFM2A</i> <i>vvFM2B</i>	<i>vvFM2A.out</i> <i>vvFM2A.sav</i> <i>vvFM2B.ou</i>	yes
1.3	Upstream saturation times a constant	<i>vvFM3A</i> <i>vvFM3B</i>	<i>vvFM3A.out</i> <i>vvFM3A.sav</i> <i>vvFM3B.out</i>	yes
1.4	Upstream relative permeability	<i>vvFM4A</i> <i>vvFM4B</i>	<i>vvFM4A.out</i> <i>vvFM4B.ou</i>	yes
1.5	Upstream relative permeability times a factor	<i>vvFM5A</i> <i>vvFM5B</i>	<i>vvFM5A.out</i> <i>vvFM5B.ou</i>	yes
2	Free drainage boundary condition	<i>vvFDBC</i>	<i>vvFDBC.out</i>	yes
3	Active Fracture Concept	<i>vv</i>	<i>vv.out</i>	yes
4.1	Modification of Brooks-Corey capillary pressure function	<i>vvv</i> <i>vv</i>	<i>vvv_ch.tec</i>	yes
4.2	Modification of van Genuchten capillary pressure function	<i>vvv</i> <i>vv</i>	<i>vvv_ch.tec</i>	yes
5	New observation types SECONDARY and HEAT FLOW	<i>vv</i> <i>vvv</i>	<i>vvv.out</i> <i>vv.out</i>	yes
6	New priorities in porosity definition	<i>vvv</i> <i>vv</i>	<i>vv.out</i>	yes
7	Adjusting array dimensions	<i>vvRITi</i> <i>vvRIT</i> <i>vvRIT.dat</i> <i>minsize.inc</i>	<i>vvRITi.out</i>	yes
8	Application control	<i>vvRITi</i> <i>vvRIT</i> <i>vvRIT.dat</i>	<i>vvRITi.out</i>	yes
9	Regression testing	<i>vvRITi</i> <i>vvRIT</i> <i>vvRIT.dat</i>	<i>vvRITi.out</i> <i>vvRIT.v30.out</i>	yes

Since all acceptance criteria are met, all functional requirements are fulfilled, i.e., ITOUGH2 V3.2 can be considered technically validated in compliance with YMP-LBNL-QIP-SI.0, Rev. 3, Mod. 0.

Acknowledgment

I would like to thank Y.-S. Wu, C. F. Ahlers, M. Bandurraga, H. H. Liu, and J. Birkholzer for their support during the development and testing of the new ITOUGH2 features discussed in this report. The review comments by C. M. Oldenburg are gratefully acknowledged. This work was supported, in part, by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc. and the Ernest Orlando Lawrence Berkeley National Laboratory, under contract No. DE-AC03-76SF00098.

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Appendix A: List of Files

=====
List of files in directory ~/itough2v3.2
=====

Contains source code and utilities of ITOUGH2 V3.2.
See file read.me for installation instructions.

-rw-r--r--	1	finster	stefan	7849	Jun 30 00:00	Makefile
-r--r--r--	1	finster	stefan	915	Jun 30 00:00	best.inc
-r--r--r--	1	finster	stefan	274	Jun 30 00:00	bfact.inc
-r--r--r--	1	finster	stefan	519	Jun 30 00:00	break.inc
-r--r--r--	1	finster	stefan	1436	Jun 30 00:00	caltim.inc
-r--r--r--	1	finster	stefan	232	Jun 30 00:00	carrera.inc
-r--r--r--	1	finster	stefan	197	Jun 30 00:00	comment.inc
-r--r--r--	1	finster	stefan	1126	Jun 30 00:00	connect.inc
-r--r--r--	1	finster	stefan	995	Jun 30 00:00	copa.inc
-r--r--r--	1	finster	stefan	496	Jun 30 00:00	covar.inc
-r--r--r--	1	finster	stefan	1039	Jun 30 00:00	data.inc
-r--r--r--	1	finster	stefan	1377	Jun 30 00:00	elements.inc
-r--r--r--	1	finster	stefan	352	Jun 30 00:00	eos.inc
-r--r--r--	1	finster	stefan	33418	Jun 30 00:00	eos1.f
-r--r--r--	1	finster	stefan	36279	Jun 30 00:00	eos2.f
-r--r--r--	1	finster	stefan	40621	Jun 30 00:00	eos3.f
-r--r--r--	1	finster	stefan	39616	Jun 30 00:00	eos3ecm.f
-r--r--r--	1	finster	stefan	52446	Jun 30 00:00	eos4.f
-r--r--r--	1	finster	stefan	35597	Jun 30 00:00	eos5.f
-r--r--r--	1	finster	stefan	42941	Jun 30 00:00	eos9.f
-r--r--r--	1	finster	stefan	46556	Jun 30 00:00	eos9ecm.f
-r--r--r--	1	finster	stefan	2628	Jun 30 00:00	estim.inc
-r--r--r--	1	finster	stefan	185	Jun 30 00:00	flcom.inc
-r--r--r--	1	finster	stefan	40	Jun 30 00:00	ff.inc
-r--r--r--	1	finster	stefan	1056	Jun 30 00:00	filename.inc
-r--r--r--	1	finster	stefan	734	Jun 30 00:00	fixsize.inc
-r--r--r--	1	finster	stefan	3244	Jun 30 00:00	flags.inc
-r--r--r--	1	finster	stefan	472	Jun 30 00:00	flovel.inc
-r--r--r--	1	finster	stefan	356	Jun 30 00:00	gasprop.inc
-r--r--r--	1	finster	stefan	236	Jun 30 00:00	gradient.inc
-r--r--r--	1	finster	stefan	677	Jun 30 00:00	guess.inc
-r--r--r--	1	finster	stefan	748	Jun 30 00:00	hyster.inc
-r--r--r--	1	finster	stefan	537	Jun 30 00:00	ifsdummy.f
-r--r--r--	1	finster	stefan	214	Jun 30 00:00	inval.inc
-rw-r--r--	1	finster	stefan	179	Jun 30 00:00	invdir
-rwxr-xr-x	1	finster	stefan	4120	Jun 30 00:00	it2help
-rw-r--r--	1	finster	stefan	239291	Jun 30 00:00	it2help.txt
-r--r--r--	1	finster	stefan	216692	Jun 30 00:00	it2input.f
-r--r--r--	1	finster	stefan	331372	Jun 30 00:00	it2main.f
-r--r--r--	1	finster	stefan	19867	Jun 30 00:00	it2user.f
-r--r--r--	1	finster	stefan	97659	Jun 30 00:00	it2xxxx.f
-r--r--r--	1	finster	stefan	416	Jun 30 00:00	iter.inc
-rwxr-xr-x	1	finster	stefan	11967	Jun 30 00:00	itough2

```

-rw-r--r-- 1 finster stefan      668 Jun 30 00:00 itough2.log
-rw-r--r-- 1 finster stefan    6599 Jun 30 00:00 itough2v32.lst
-r--r--r-- 1 finster stefan      544 Jun 30 00:00 jacobi.inc
-rwxr-xr-x 1 finster stefan    3805 Jun 30 00:00 kit
-r--r--r-- 1 finster stefan      298 Jun 30 00:00 levmar.inc
-r--r--r-- 1 finster stefan      723 Jun 30 00:00 lineq.inc
-r--r--r-- 1 finster stefan  114512 Jun 30 00:00 ma28.f
-r--r--r-- 1 finster stefan      571 Jun 30 00:00 maxm.inc
-rw-r--r-- 1 finster stefan     4510 Jun 30 00:00 maxsize.inc
-rw-r--r-- 1 finster stefan     4510 Jun 30 00:00 maxsize0.inc
-r--r--r-- 1 finster stefan    11073 Jun 30 00:00 mdepccray.f
-r--r--r-- 1 finster stefan    11217 Jun 30 00:00 mdepdec.f
-r--r--r-- 1 finster stefan    11070 Jun 30 00:00 mdepfp.f
-r--r--r-- 1 finster stefan    11053 Jun 30 00:00 mdepibm.f
-r--r--r-- 1 finster stefan     4212 Jun 30 00:00 mdeplah.f
-r--r--r-- 1 finster stefan    11315 Jun 30 00:00 mdepsgi.f
-r--r--r-- 1 finster stefan    11247 Jun 30 00:00 mdepsun.f
-r--r--r-- 1 finster stefan    50718 Jun 30 00:00 meshm.f
-r--r--r-- 1 finster stefan     894 Jun 30 00:00 meshm.inc
-r--r--r-- 1 finster stefan    4487 Jun 30 00:00 minsize.inc
-r--r--r-- 1 finster stefan     376 Jun 30 00:00 mn.inc
-r--r--r-- 1 finster stefan     129 Jun 30 00:00 nstl.inc
-r--r--r-- 1 finster stefan    3043 Jun 30 00:00 obser.inc
-r--r--r-- 1 finster stefan    2029 Jun 30 00:00 param.inc
-r--r--r-- 1 finster stefan    1341 Jun 30 00:00 parsel.inc
-r--r--r-- 1 finster stefan     465 Jun 30 00:00 penalty.inc
-r--r--r-- 1 finster stefan     545 Jun 30 00:00 plot.inc
-r--r--r-- 1 finster stefan    1055 Jun 30 00:00 primary.inc
-rwxr-xr-x 1 finster stefan    5272 Jun 30 00:00 prista
-r--r--r-- 1 finster stefan     247 Jun 30 00:00 probsize.inc
-r--r--r-- 1 finster stefan     557 Jun 30 00:00 ratesave.inc
-r--r--r-- 1 finster stefan     422 Jun 30 00:00 rconst.inc
-rw-r--r-- 1 finster stefan   13611 Jun 30 00:00 read.me
-r--r--r-- 1 finster stefan     298 Jun 30 00:00 resid.inc
-r--r--r-- 1 finster stefan     612 Jun 30 00:00 rmasvol.inc
-r--r--r-- 1 finster stefan    1375 Jun 30 00:00 rock.inc
drwxrwxrwx 2 finster stefan     512 Jun 30 00:00 sampleQA
-r--r--r-- 1 finster stefan     490 Jun 30 00:00 second.inc
-r--r--r-- 1 finster stefan     887 Jun 30 00:00 siman.inc
-r--r--r-- 1 finster stefan     297 Jun 30 00:00 skinrad.inc
-r--r--r-- 1 finster stefan     401 Jun 30 00:00 stocha.inc
-r--r--r-- 1 finster stefan    65050 Jun 30 00:00 t2cg1.f
-r--r--r-- 1 finster stefan  164873 Jun 30 00:00 t2f.f
-r--r--r-- 1 finster stefan     748 Jun 30 00:00 t2voc.inc
-r--r--r-- 1 finster stefan     123 Jun 30 00:00 title.inc
-rwxr-xr-x 1 finster stefan    1752 Jun 30 00:00 tough2
-r--r--r-- 1 finster stefan    1807 Jun 30 00:00 units.inc
-r--r--r-- 1 finster stefan     211 Jun 30 00:00 usercom.inc
-r--r--r-- 1 finster stefan     178 Jun 30 00:00 weight.inc
-r--r--r-- 1 finster stefan    2238 Jun 30 00:00 wells.inc
-r--r--r-- 1 finster stefan     274 Jun 30 00:00 xuser.inc

```

Total: 93 files + 1 subdirectory

=====
List of files in directory ~/itough2v3.2/sampleQA
=====

Contains input files for running validation problems described in:

ITOUGH2 V3.2, Verification and Validation Report

Report LBNL-42002, Lawrence Berkeley National Laboratory, Berkeley,
Calif.

June 1998

-rwxr-xr-x 1 finster stefan 4487 Jun 29 09:34 minsize.inc
-rw-r--r-- 1 finster stefan 2573 Jun 29 09:34 vv
-rw-r--r-- 1 finster stefan 2052 Jun 29 09:34 vvFDBC
-rw-r--r-- 1 finster stefan 3751 Jun 29 09:34 vvFM1A
-rw-r--r-- 1 finster stefan 3791 Jun 29 09:34 vvFM1B
-rw-r--r-- 1 finster stefan 3723 Jun 29 09:34 vvFM2A
-rw-r--r-- 1 finster stefan 3842 Jun 29 09:34 vvFM2B
-rw-r--r-- 1 finster stefan 3760 Jun 29 09:34 vvFM3A
-rw-r--r-- 1 finster stefan 3866 Jun 29 09:34 vvFM3B
-rw-r--r-- 1 finster stefan 3720 Jun 29 09:34 vvFM4A
-rw-r--r-- 1 finster stefan 3835 Jun 29 09:34 vvFM4B
-rw-r--r-- 1 finster stefan 3760 Jun 29 09:34 vvFM5A
-rw-r--r-- 1 finster stefan 3857 Jun 29 09:34 vvFM5B
-rw-r--r-- 1 finster stefan 1724 Jun 29 09:34 vvRIT
-rw-r--r-- 1 finster stefan 3219 Jun 29 09:34 vvRIT.dat
-rw-r--r-- 1 finster stefan 2724 Jun 29 09:34 vvRITi
-rw-r--r-- 1 finster stefan 3599 Jun 29 09:34 vvi

Total 17 files

Appendix B: File *read.me*

.....READ.ME.....READ.ME.....READ.ME.....READ.ME.....

```
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@
@ @@@ @@@@@ @@ @ @ @@@ @ @ @@@@ @
@ @ @ @ @ @ @ @ @ @ @ @ @ @
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@ @ @ @ @ @ @ @ @ @ @ @ @ @
@ @@@ @ @ @ @ @ @ @ @ @ @ @ @
@
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

This flyer contains brief instructions for installing and running ITOUGH2 under UNIX operating system. Machine-dependent routines are provided for the various computer systems. Installing ITOUGH2 on another computer system may require minor modifications of the subroutines provided in file <mdep???.f>.

ITOUGH2 can also be compiled on a PC. If the Lahey Compiler is used, the appropriate compiler options and machine-dependent subroutines are provided in files Makefile and mdeplah.f, respectively.

The distribution includes the source code, various utility script files, and sample problems:

Utilities

- (1) read.me - The file you are reading.
- (2) Makefile - UNIX makefile for compiling and linking ITOUGH2.
- (3) itough2 - UNIX script file for running ITOUGH2.
(in subdirectory ../bin).
See header of file for details.
- (4) tough2 - UNIX script file for running TOUGH2 as a dummy
ITOUGH2 run.
(put in subdirectory ../bin).
See header of file for details.
- (5) prista - UNIX scrip file for displaying status of ITOUGH2
run.
(put in subdirectory ../bin).
See header of file for details.
- (6) kit - UNIX script file for sending signals to ITOUGH2.

(put in subdirectory ../bin).
See header of file for details.

- (7) it2help - UNIX script file for displaying ITOUGH2 manual pages
(put in subdirectory ../bin).
See header of file for details.
- (8) it2help.txt - ITOUGH2 manual pages.
- (9) invdir - Dummy ITOUGH2 input file to solve direct problem
only.

ITOUGH2 FORTRAN source files

- (10) *.inc - Include files containing COMMON blocks and PARAMETER
statements for dimensioning major arrays
(see maxsize.inc).
- (11) it2main.f - ITOUGH2 main subroutines.
- (12) it2input.f - Subroutines reading ITOUGH2 input file.
- (13) it2user.f - Subroutines for user-specified parameters, user-
specified observations, user-specified boundary
conditions, and user-specified data functions.
- (14) it2xxxx.f - Subroutines for minimization algorithm,
matrix operations, eigenanalysis, etc.
- (15) mdep???.f - Machine-dependent subroutines for ???
??? = ibm, dec, sun, hp, sgi, star, lah, cray.

TOUGH2 FORTRAN source files

- (16) t2cg1.f - Conjugate gradient solvers.
- (17) t2f.f - Core module of TOUGH2.
- (18) meshm.f - Module with internal mesh generation facilities.
- (19) eos#.f - Equation of state module No. #.
- (20) ma28.f - Direct linear equation solver.

Sample problems (subdirectory <sampleQA>)

+++++

INSTALLATION

+++++

Installing ITOUGH2 requires basic knowledge about the UNIX operating system, including shell programming, the makefile utility, changing permissions, and adding a directory to the PATH shell variable. If ITOUGH2 is installed exactly as recommended below, only very minor modifications have to be made to the Makefile and the script files, if at all.

- (1) Create a new directory in your home directory. Type:
`cd ; mkdir itough2`

Multiple ITOUGH2 versions can be installed in subdirectories `itough2v?` where `?` is the version number used with the `-v` option on the `itough2` command line.

- (2) Move the compressed tar file `it2_tar.Z` to directory `~/itough2` or `~/itough2v?:`
`mv it2_tar.Z itough2`

- (3) Go to the newly created directory and uncompress the tar file. Type:
`cd itough2 ; uncompress it2_tar.Z`

- (4) Extract the files from the archive file. Type:
`tar -xvf it2_tar`

A subdirectory `~/itough2/samples` is created containing all the sample problems. The script files (`tough2`, `itough2`, `prista`, `it2help`, and `kit`) are copied to subdirectory `../bin`.

- (5) If you want to change the dimensions of the major TOUGH2 and ITOUGH2 arrays, edit file `<maxsize.inc>`.

- (6) Edit file `<Makefile>` to customize the following variables:

`EOS = ?` : Provide number of the EOS module being used.
`COM = ?` : Provide name of the computer system being used.
Possibilities: `ibm`, `sun`, `star`, `sgi`, `dec`, and `hp`.
`FOR = ?` : name of FORtran compiler.
`COO = ?` : Provide COmpiler Options for compilation.
`LIN = ?` : Provide specific LINker options if required.

Compiler options are provided for IBM, SUN, DEC ALPHA, and HP workstations. Select the appropriate block by deleting the #-sign in the first column before `COM`, `FOR`, `COO`, (and `LIN`), and put #-signs elsewhere.

- (7) If user-specified functions are required, they have to be programmed into the appropriate subroutine in file `<it2user.f>` (see examples therein and in the ITOUGH2 Command Reference).

- (8) Customize ITOUGH2, if needed, in particular:
Set default plotting interface, variable IPLOTFMT in BLOCK DATA IT,
file <it2main.f> (default: TECPLOT).
- (9) Type "make" to run the Makefile. This compiles and links ITOUGH2.
The name of the executable is <itough2_IEOS.out>, where IEOS is an
integer indicating which EOS module is being used.
- (10) On SUN and DEC ALPHA workstations, you may run into a severe
linking error due to multiply defined subroutines.
However, these compilers nevertheless create a file
<itough2_IEOS.out>. This file is not executable. Type "make x" to
make it executable.
- (11) Add subdirectory ~/bin to the command search path
(if not yet defined)
Add the following line to your ~/.cshrc file:
set path =(\$PATH ~/bin).
In your home directory, type:
source ~/.cshrc
- (12) Make sure the five script files <tough2>, <itough2>, <prista>,
<kit>, and <it2help> in directory ../bin are executable.
If not, go to directory ~/itough2 and type:
make x
- (13) You may have to customize script files <prista> and <kit>.
See instructions therein.
- (14) Check appropriate installation of script files:
Go to directory ~/itough2/samples, and type "prista" or "kit".
A message will appear saying that no ITOUGH2 run is in progress.
Type "tough2" or "itough2" without any arguments. The command usage
should be printed.
- (15) The executable <itough2_IEOS.out> can also be used to run TOUGH2,
i.e., to solve the forward problem without optimization.
Running TOUGH2 as a dummy ITOUGH2 simulation assures that the same
version is used to solve both the direct and the inverse problem.
Furthermore, disk space can be saved since no separate TOUGH2
executable is needed.
A dummy ITOUGH2 input file <invdir> is provided, as well as a UNIX
script file <tough2>.
Customize script file <tough2>, if needed:
script_dir = ? : Provide path to script file <itough2>.
Default: ~/bin

RUNNING ITOUGH2

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- (1) Prepare a TOUGH2 and an ITOUGH2 input deck according to the user's guides. On-line support is provided through command `it2help` or on the Web at <http://www-esd.lbl.gov/ITOUGH2> (click on Command Index). To run ITOUGH2 type:

```
itough2 inv_file dir_file IEOS &
```

where:

- `itough2` is the command name of the script file (or alias)
- `inv_file` is the file name of the ITOUGH2 input file
- `dir_file` is the file name of the TOUGH2 input file
- `IEOS` is the number of the EOS module being used

Additional options are available; type "`itough2`" without any arguments for a list. In order to run the first sample problem, go to subdirectory `~/itough2v3.2/sampleQA` and type:

```
itough2 vvRITi vvRIT 3 &
```

It is important to add the "&" at the end of the command line. This sends the execution of the script file to the background, which allows you to use `prista` and `kit`.

The `<itough2>` script file generates a temporary directory `~/it2_PID`.

All files are then copied into this temporary directory. ITOUGH2 is executed, and the result files are copied back to your working directory. This allows one to run multiple inversions at the same time without generating conflicting file names.

- (2) During execution, the status of the inverse modeling run can be displayed by running the `<prista>` script file. Follow the instructions on screen.
- (3) If you wish to prematurely terminate an ITOUGH2 simulation or to send a signal which triggers a specific action (e.g. provides printout), use the `<kit>` script file and follow the instructions on screen.

Running TOUGH2

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- (1) Prepare a TOUGH2 input deck.
- (2) Type "`tough2 dir_file IEOS &`" for execution, where:
 - `tough2` is the command name of the script file (or alias)
 - `dir_file` is the file name of the TOUGH2 input deck
 - `IEOS` is the number of the EOS module being used

Additional options are available; type "`tough2`" without any arguments for a list.

Debugging

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Run the sample problems to check the proper installation of the code.

If no results are obtained, check:

- (1) whether the script file <itough2> is executable and accessible from your working directory;
- (2) whether the ITOUGH2 executable <itough2_3.out> exists;
- (3) whether the path name to the ITOUGH2 executable is correct (see shell variable prog_dir in script file <itough2>);
- (4) error messages in the ITOUGH2 output file;
- (5) error messages in the TOUGH2 output file;
- (6) for error messages from the shell script (files *.msg);

You may also rerun the sample problem using the -no_delete option, and examine all the files in the temporary directory ~/it2_PID.

SUGGESTIONS

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The following procedure is suggested:

- (1) Use option ">>> stop after INPUT" to check ITOUGH2 input without starting the optimization; check printout of input data; resolve errors and warnings.
- (2) Use option ">>> solve FORWARD problem only" to run one forward calculation; check whether the TOUGH2 simulation was terminated normally; draw curves of measured and computed output (see plotfile <*.tec>); check whether the initial guess was reasonable and whether the units and signs of your data were correct; check CPU time needed for one forward calculation.
- (3) Perform one iteration (">>> number of ITERATIONS: 1") and check the sensitivity coefficients; if certain parameters are not sensitive or highly correlated with other parameters, try to define new lumped parameters, or exclude the parameter from the optimization. Use option ">>> automatic parameter SELECTION" for a faster and more stable optimization.
- (4) Perform optimization; set maximum number of iterations between 5 and 15.
- (5) Carefully read warning and error messages in the ITOUGH2 output file.

(6) Please report code errors to the code developers.

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TOUGH2 is documented in:

- K. Pruess, TOUGH2 - A General Purpose Numerical Simulator for Multiphase Fluid and Heat Flow, Lawrence Berkeley Laboratory Report LBL-29400, May 1991.
- K. Pruess, TOUGH User's Guide, Lawrence Berkeley Laboratory Report LBL-20700 June 1987 (also available as Nuclear Regulatory Commission Report NUREG/CR-4645)

ITOUGH2 is documented in:

- S. Finsterle, ITOUGH2 User's Guide, Lawrence Berkeley National Laboratory, Report LBNL-40040, 1998.
- S. Finsterle, ITOUGH2 Command Reference, Lawrence Berkeley National Laboratory, Report LBNL-40041, 1997.
- S. Finsterle, ITOUGH2 Sample Problems, Lawrence Berkeley National Laboratory, Report LBNL-40042, 1997.

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