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ITOUGH2 V3.2

Verification and Validation Report

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Table of Contents

1. Introduction 1
2. Test Results 2
2.1 Fracture-Matrix Interface Area Reduction 2
2.1.1 Interface Area Reduce by a Constant 5
2.1.2 Interface Area Reduce by Upstream Saturation 6
2.1.3 Interface Area Reduce by Upstream Saturation Times a Constant 8
2.1.4 Interface Area Reduce by Upstream Relative Permeability 10
2.1.5 Interface Area Reduce by Upstream Relative Permeability Times a Constant 12

2.2 Free Drainage Boundary Condition 14
2.3 Active Fracture Concept 16
2.4 Modification to Capillary Pressure Functions 21
2.4.1 Modification to Brooks-Corey Capillary Pressure Function 21
2.4.2 Modification to van Genuchten Capillary Pressure Function 23

2.5 New Observation Types 25
2.6 New Priorities in Assigning Porosities 32
2.7 Adjusting Array Dimensions 33
2.8 Application Control 38
2.9 Regression Testing 44

3. Summary 46

Acknowledgment 47

References 47

Appendix A: List of files 48

Appendix B: File *read.me* 51

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 [*ITOUGH2 V3.0 DF6 R00*].

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
                        1.7300    0.2500
    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   1.0E-12       2.0     900.0
                        1.7300    0.2500
    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   1.0E-16       2.0     900.0
                        1.7300    0.2500                          0.01       0.1
    7         0.2000    0.1500    1.0000
    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 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 *vvFM1A*; 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 *vvFM1B*; 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:

```
tough2 -v 3.2 vvFM1A 9 &
tough2 -v 3.2 vvFM1B 9 &
```

Inspection of the two output files *vvFM1A.out* and *vvFM1B.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 *vvFM1B*, 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:

```
tough2 -v 3.2 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 0.0000000000000E+00
M   1             0.10000000E+00
 0.8921064332228E+00 0.0000000000000E+00
F   2             0.10000000E+00
 0.6098054293383E+00 0.0000000000000E+00
M   2             0.10000000E+00
 0.8960659745952E+00 0.0000000000000E+00
F   3             0.10000000E+00
 0.2750228155389E+00 0.0000000000000E+00
M   3             0.10000000E+00
 0.9881525567958E+00 0.0000000000000E+00
F   4             0.10000000E+00
 0.1754130794552E+00 0.0000000000000E+00
M   4             0.10000000E+00
 0.9890779950707E+00 0.0000000000000E+00
F   5             0.10000000E+00
 0.2000000000000E-01 0.0000000000000E+00
M   5             0.10000000E+00
 0.9900000000000E+00 0.0000000000000E+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+000.5000E+000.43389087
F   2M   2                   10.0000E+000.5000E+000.60980543
F   3M   3                   10.0000E+000.5000E+000.27502282
F   4M   4                   10.0000E+000.5000E+000.17541308
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 2.1.2.2. 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:

```
tough2 -v 3.2 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:

```
tough2 -v 3.2 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 0.0000000000000E+00
M   1             0.10000000E+00
 0.8357579578799E+00 0.0000000000000E+00
F   2             0.10000000E+00
 0.6175860651419E+00 0.0000000000000E+00
M   2             0.10000000E+00
 0.8436032656234E+00 0.0000000000000E+00
F   3             0.10000000E+00
 0.2911632608216E+00 0.0000000000000E+00
M   3             0.10000000E+00
 0.9878238253713E+00 0.0000000000000E+00
F   4             0.10000000E+00
 0.1852263062714E+00 0.0000000000000E+00
M   4             0.10000000E+00
 0.9889180282040E+00 0.0000000000000E+00
F   5             0.10000000E+00
 0.2000000000000E-01 0.0000000000000E+00
M   5             0.10000000E+00
 0.9900000000000E+00 0.0000000000000E+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:

```
tough2 -v 3.2 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:

```
tough2 -v 3.2 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.

```
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
Case 4: Fracture-Matrix Interface Area Reduction: upstream rel. perm.

                              KCYC =   36  -  ITER =    1  -  TIME = 0.42950E+16

 ELEM.  INDEX   X1          DX1        K(LIQ.)
 F    1      1 0.43804E+00 0.00000E+00 0.63542E-02
 M    1      2 0.82310E+00 0.00000E+00 0.14249E-01
 F    2      3 0.61830E+00 0.00000E+00 0.34911E-01
 M    2      4 0.83338E+00 0.00000E+00 0.16522E-01
 F    3      5 0.29271E+00 0.00000E+00 0.92665E-03
 M    3      6 0.98779E+00 0.00000E+00 0.16919E+00
 F    4      7 0.18617E+00 0.00000E+00 0.10746E-03
 M    4      8 0.98890E+00 0.00000E+00 0.17829E+00
 F    5      9 0.20000E-01 0.00000E+00 0.26158E-09
 M    5     10 0.99000E+00 0.00000E+00 0.18831E+00

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

Figure 2.1.4.1. Excerpt from file *vvFM4A.out*, showing steady-state liquid relative permeabilities obtained in Run A.

```
CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1M   1                    10.0000E+000.5000E+000.63542E-2
F   2M   2                    10.0000E+000.5000E+000.34911E-1
F   3M   3                    10.0000E+000.5000E+000.92665E-3
F   4M   4                    10.0000E+000.5000E+000.10746E-3
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 2.1.4.2. Block CONNE of file *vvFM4B*, showing interface areas reduced by the fracture relative permeabilities shown in Figure 2.1.4.1.

The following command line was used for Run B:

```
tough2 -v 3.2 vvFM4B 9 &
```

Inspection of the two output files *vvFM4A.out* and *vvFM4B.out* confirms that identical results were obtained, fulfilling Requirement 1.4.

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:

```
tough2 -v 3.2 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.

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

Case 5: Fracture-Matrix Interface Area Reduction: upstream rel. perm.*factor

                                      KCYC =    35  -  ITER =     1  -  TIME = 0.53687E+16

 ELEM.  INDEX    X1          DX1         K(LIQ.)
 F    1      1 0.43834E+00 0.00000E+00 0.63752E-02
 M    1      2 0.80758E+00 0.00000E+00 0.11399E-01
 F    2      3 0.61896E+00 0.00000E+00 0.35104E-01
 M    2      4 0.81769E+00 0.00000E+00 0.13182E-01
 F    3      5 0.29408E+00 0.00000E+00 0.94738E-03
 M    3      6 0.98776E+00 0.00000E+00 0.16894E+00
 F    4      7 0.18700E+00 0.00000E+00 0.10976E-03
 M    4      8 0.98889E+00 0.00000E+00 0.17815E+00
 F    5      9 0.20000E-01 0.00000E+00 0.26158E-09
 M    5     10 0.99000E+00 0.00000E+00 0.18831E+00

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

Figure 2.1.5.1. Excerpt from file *vvFM5A.out*, showing steady-state liquid relative permeabilities obtained in Run A.

```
CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F    1M    1                   10.0000E+000.5000E+000.63752E-3
F    2M    2                   10.0000E+000.5000E+000.35104E-2
F    3M    3                   10.0000E+000.5000E+000.94738E-4
F    4M    4                   10.0000E+000.5000E+000.10976E-4
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 2.1.5.2. Block CONNE of file *vvFM5B*, showing interface areas reduced by 10% of the fracture liquid relative permeabilities shown in Figure 2.1.5.1.

The following command line was used for Run B:

```
tough2 -v 3.2 vvFM5B 9 &
```

Inspection of the two output files *vvFM5A.out* and *vvFM5B.out* confirms that identical results were obtained, fulfilling Requirement 1.5.

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:

```
tough2 -v 3.2 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                              0.01       0.1
    7         0.5000    0.0100 1.000E-04                 1.000
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                              0.01       0.1
    7         0.5000    0.0100 1.000E-04                 1.000

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.

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

  TOTAL TIME      KCYC  ITER  ITERC   KON      DX1M          DX2M          DX3M         MAX. RES.      NER   KER          DELTEX
  0.67109E+14      25     1     54      2   0.00000E+00  0.00000E+00  0.00000E+00   0.53937E-05       4     1        0.33554E+14

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

 ELEM.  INDEX   PRES        S(liq)      PCAP         K(rel)      DIFFUS.          PERM    POROSITY AIR_ENTRY_P.
                 (PA)                    (PA)                      (m^2/s)

 F    1      1 0.10130E+06 0.30687E+00 -.31813E+05 0.11598E-02 0.12022E-05 0.10000E-11 0.10000E+00 0.10000E-01
 F    2      2 0.10130E+06 0.30687E+00 -.31813E+05 0.11598E-02 0.12022E-05 0.10000E-11 0.10000E+00 0.10000E-01
 F    3      3 0.10130E+06 0.30687E+00 -.31813E+05 0.11598E-02 0.12022E-05 0.10000E-11 0.10000E+00 0.10000E-01
 F    4      4 0.10130E+06 0.30687E+00 -.31813E+05 0.11598E-02 0.12022E-05 0.10000E-11 0.10000E+00 0.10000E-01
 F    5      5 0.10130E+06 0.50000E+00 -.17556E+05 0.12088E-01 0.50495E-05 0.10000E-11 0.10000E+00 0.10000E-01

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

Figure 2.2.2. Excerpt from TOUGH2 output file *vvFDBC.out*, showing uniform saturation profile despite capillary pressure gradient at the bottom of the column.

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:

$$f_a = S_e^{\gamma} \tag{2.3.1}$$

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

$$S_e = \frac{S_l - S_{lr}}{1 - S_{lr}} \tag{2.3.2}$$

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:

$$S_{ea} = \frac{S_e}{f_a} = S_e^{1-\gamma} \tag{2.3.3}$$

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

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

and

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

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

$$a_{fm} = S_e^{1+\gamma} \tag{2.3.6}$$

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                           0.3
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                           0.3

PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3   1        11000080100000000400001000
                            1.0

                1.0E5                10.3                20.0
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    3    2    6
ELEME----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
                1.1E5                10.3                50.0
ELM 2                        0.5
                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:

$$q_{ELM2-ELM1} = -k \cdot A \cdot a_{fm} \frac{k_{rl}}{\mu_l} \rho_l \left(\frac{p_{ELM1} - p_{ELM2}}{d_1 + d_2} \right)$$

$$= -10^{-12} \cdot 0.1 \cdot 0.5443 \frac{0.13177}{5.4418 \cdot 10^{-4}} 988.07 \left(\frac{1.0704 \cdot 10^5 - 1.0002 \cdot 10^5}{0.05 + 0.05} \right)$$

$$= -9.142 \cdot 10^{-4} \, kg / s$$

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)                                                          (PA)        (PA)       (KG/M**3)   (KG/M**3)

 ELM 1      1 0.10775E+06 0.49999E+02 0.30002E+00 0.69998E+00 0.92531E+00 0.15337E-04 0.12335E+05 -.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 -.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 -.10956E+04 0.11783E+01 0.99832E+03
 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

          TOUGH2 input file for V&V of:

                                                                                       KCYC =    1  -  ITER =    3  -  TIME = 0.10000E+01
0         ELEM1  ELEM2  INDEX     FLOH       FLOH/FLOF        FLOF        FLO(GAS)     FLO(LIQ.)   VEL(GAS)     VEL(LIQ.)
                                   (W)        (J/KG)         (KG/S)        (KG/S)       (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:

                                                                                       KCYC =    1  -  ITER =    3  -  TIME = 0.10000E+01
 ELEM.  INDEX   X1          X2          X3          DX1         DX2         DX3         K(GAS)      K(LIQ.)      H(GAS)      H(LIQ.)
                                                                                                                  (J/KG)      (J/KG)

 ELM 1      1 0.10775E+06 0.10300E+02 0.49999E+02 -.22506E+04 0.23491E-04 -.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 -.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 -.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 $0 \le S_l \le 1$ 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):

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

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

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

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

$$p_c \ge -p_{c,\max} \qquad (2.4.1.3)$$

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

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

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

Table 2.4.1.1. Input Parameters for Modified Brooks-Corey Model

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

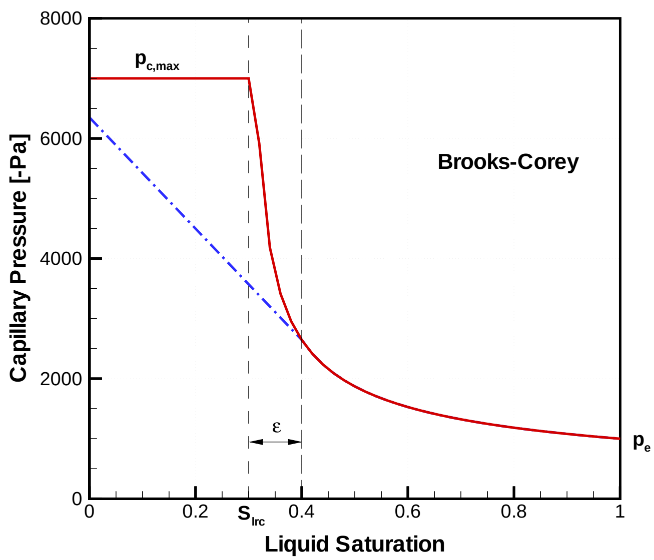

Figure 2.4.1.1. Modified Brooks-Corey capillary pressure curves.

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):

$$S_{ec} = \frac{S_l - S_{lrc}}{1 - S_{lrc}} \tag{2.4.2.1a}$$

$$S_{ek} = \frac{S_l - S_{lrk}}{1 - S_{lrk} - S_{gr}} \tag{2.4.2.1b}$$

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

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

$$p_c \geq -p_{c,\max} \tag{2.4.2.3}$$

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

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

$$k_{rg} = 1 - k_{rl} \tag{2.4.2.4c}$$

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) ≥ 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.

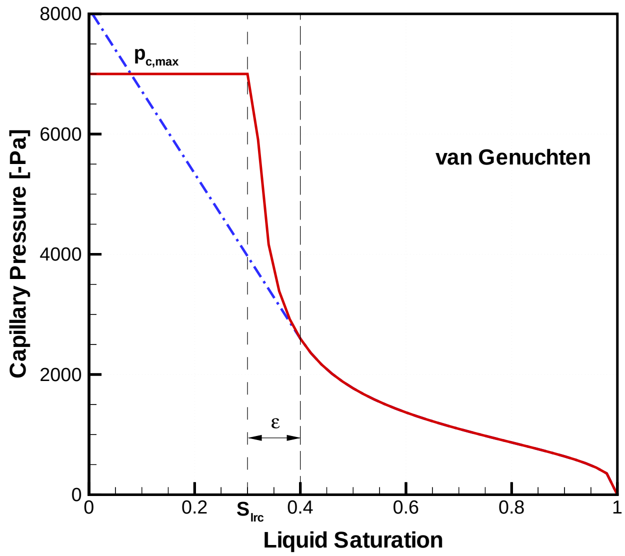

Figure 2.4.2.1. Modified van Genuchten capillary pressure curves.

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=Xwl
         >>>> LIQUID PHASE
         >>>> PARAMETER : 7
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 2,8=Xal
         >>>> 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.

```
 SECONDARY PARAMETERS

 ELEMENT ELM 1
 0.300023E+00 0.868225E+00 0.190691E-04 0.111143E+01 0.313374E+06 0.000000E+00 0.746918E-01 0.925308E+00 0.699977E+00 0.131775E+00
 0.544175E-03 0.988072E+03 0.209335E+06 -.707148E+03 0.999985E+00 0.153374E-04 0.499994E+02 0.000000E+00

...

 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)                                                        (PA)        (PA)       (KG/M**3)   (KG/M**3)

 ELM 1      1 0.10775E+06 0.49999E+02 0.30002E+00 0.69998E+00 0.92531E+00 0.15337E-04 0.12335E+05 -.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 -.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 -.10956E+04 0.11783E+01 0.99832E+03
 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

         TOUGH2 input file for V&V of:

                                                                                   KCYC =    1  -  ITER =    3  -  TIME = 0.10000E+01
         ELEM1  ELEM2  INDEX    FLOH       FLOH/FLOF       FLOF        FLO(GAS)     FLO(LIQ.)   VEL(GAS)     VEL(LIQ.)
                                 (W)         (J/KG)       (KG/S)        (KG/S)       (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:

                                                                                   KCYC =    1  -  ITER =    3  -  TIME = 0.10000E+01
 ELEM.  INDEX   X1          X2          X3          DX1         DX2         DX3        K(GAS)     K(LIQ.)     H(GAS)      H(LIQ.)
                                                                                                             (J/KG)      (J/KG)

 ELM 1      1 0.10775E+06 0.10300E+02 0.49999E+02 -.22506E+04 0.23491E-04 -.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 -.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 -.69924E-05 0.33025E-05 0.24311E+00 0.13583E+00 0.13462E+06 0.83954E+05
0@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

Figure 2.5.2. Excerpt from TOUGH2 output file *vv.out*, showing secondary parameters, mass fractions, relative permeabilities, capillary pressure, and heat flux.

```
==========================================================================================================================================
                                                        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 *vvi* (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
      INTEGER MAXTIM
      PARAMETER (MAXTIM=61)
C
C ********************************************************************
C TOUGH2 parameter statements
C ********************************************************************
C
C --- MAXEL    : Maximum number of elements
      INTEGER MAXEL
      PARAMETER (MAXEL=53)
C
C --- MAXCON   : Maximum number of connections
      INTEGER MAXCON
      PARAMETER (MAXCON=52)
C
C --- MAXK     : Maximum number of components/species
      INTEGER MAXK
      PARAMETER (MAXK=2)
C
C --- MAXEQ    : Maximum number of equations per block
      INTEGER MAXEQ
      PARAMETER (MAXEQ=3)
C
C --- MAXPH    : Maximum number of phases
      INTEGER MAXPH
      PARAMETER (MAXPH=2)
C
C --- MAXB     : Maximum number of phase-dependent secondary variables
C                other than component mass fractions
      INTEGER MAXB
      PARAMETER (MAXB=6)
C
C --- MAXSS    : Maximum number of sources/sinks
      INTEGER MAXSS
      PARAMETER (MAXSS=1)
C
C --- MAVTAB   : Maximum average number of table entries per sink/source
      INTEGER MAVTAB
      PARAMETER (MAVTAB=1)
C
C --- MAXROC   : Maximum number of rock types
      INTEGER MAXROC
      PARAMETER (MAXROC=3)
C
C --- MAXTSP   : Maximum number of specified time steps divided by 8
      INTEGER MAXTSP
      PARAMETER (MAXTSP=1)
C
C --- MAXLAY   : Maximum number of reservoir layers for deliverability
      INTEGER MAXLAY
      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!).
      INTEGER MXRPCP
      PARAMETER (MXRPCP=7)
C
C --- MXPCTB   : Maximum points in table of ECM capillary pressure
C                vs. saturation
      INTEGER MXPCTB
      PARAMETER (MXPCTB=1)
C
C --- MXTBC    : Maximum number of elements with time vs. boundary condition
C --- MXTBPT   : Maximum number of time vs. pressure data
      INTEGER MXTBC,MXTBPT
      PARAMETER (MXTBC=1)
      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.
       INTEGER LICN,LIRN
       PARAMETER (LIRN=2*(MAXEL+2*MAXCON)*MAXEQ*MAXEQ)
       PARAMETER (LICN=4*(MAXEL+2*MAXCON)*MAXEQ*MAXEQ)
C
C --- Parameters for conjugate gradient package t2cg1
       INTEGER NREDM,MNZ,NRWORK,NIWORK
       PARAMETER (NREDM=MAXEQ*MAXEL)
       PARAMETER (MNZ=(MAXEL+2*MAXCON)*MAXEQ*MAXEQ)
       PARAMETER (NRWORK=1000+MNZ+38*NREDM)
       PARAMETER (NIWORK=32+MNZ+5*NREDM)
C
C --- Parameters for IFS
C      MAXIFSP  : Maximum number of IFS parameters
       INTEGER MAXIFSP
       PARAMETER (MAXIFSP=1)
C
C ***********************************************************************
C ITOUGH2 parameter statements
C ***********************************************************************
C --- MAXN      : Maximum number of parameters to be estimated
       INTEGER MAXN
       PARAMETER (MAXN=3)
C
C --- MAXO      : Maximum number of datasets
       INTEGER MAXO,MAXOTWO
       PARAMETER (MAXO=2)
       PARAMETER (MAXOTWO=2*MAXO)
C
C --- MAXM      : Maximum number of calibration points
C      (approx. number of datasets times number of calibration times)
       INTEGER MAXM
       PARAMETER (MAXM=123)
C
C --- MAXPD     : Max number of paired data
       INTEGER MAXPD
       PARAMETER (MAXPD=120)
C
C --- MAXR      : Dimension of array RPAR and IPAR, ROBS and IOBS
       INTEGER MAXR
       PARAMETER (MAXR=10)
C
C --- MAXBRK    : Max number of points in time at which SAVE file is written (restart)
       INTEGER MAXBRK
       PARAMETER (MAXBRK=1)
C
C --- MAXEBRK   : Max number of elements with new initial conditions after break
       INTEGER MAXEBRK
       PARAMETER (MAXEBRK=1)
C
C --- MAXCOEFF : Max number of coefficients for data modeling functions
       INTEGER MAXCOEFF
       PARAMETER (MAXCOEFF=1)
C
C --- MAXMCS    : Max number of Monte Carlo simulations
       INTEGER MAXMCS
       PARAMETER (MAXMCS=1)
C
C --- MAXCURVE : Max number of curves to be plotted
       INTEGER MAXCURVE
       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.

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

V3.2 (May 1998) FOR SUN WORKSTATION, S. FINSTERLE


=====================================================================================================================
                                  >>>>>>>>>>>>> 25-Jun-98  10:48 <<<<<<<<<<<<<
=====================================================================================================================
ITOUGH2 INPUT FILE             :  vvRITi
TOUGH2 INPUT FILE              :  vvRIT
DIRECTORY                      :  /m/presto/u/finster/itough2v3.2/TestCases
EQUATION OF STATE MODULE NO.   :  3 - Two-phase, non-isothermal flow of water and air
COMPONENTS                     :  WATER     AIR       HEAT
PHASES                         :  GAS       LIQUID
TOUGH2 TITLE                   :  TOUGH2 input file for simulating two-phase,transient 'Darcy' experiment
=====================================================================================================================
```

Figure 2.8.1. Excerpt from ITOUGH2 output file *vvRITi.out*, showing starting date, input file names, directory, and number of equation-of-state module used.

```
COMPUTER SYSTEM
===============

Machine type                                    : SUN Workstation
UNIX script file name                           : /m/presto/u/finster/bin/itough2
UNIX command line arguments                     : -v 3.2 vvRITi vvRIT 3
Host name                                       : presto.lbl.gov
User name                                       : finster
Executable                                      : /m/presto/u/finster/itough2v3.2/itough2_3.presto.lbl.gov
Computer is as fast as a SUN ULTRA1


--- End of ITOUGH2 input job:   86 lines read,    0.32 CPU-seconds used
```

Figure 2.8.2. Excerpt from ITOUGH2 output file *vvRITi.out*, showing information regarding computer system used and command line arguments.

```
=====================================================================================================
     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 indicesof 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
    INPARAME 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
LEVMAR   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
RELP     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
                                          CAN CALL MA28 OR A PACKAGE OF CONJUGATE GRADIENT SOLVERS
CONVER   2.5      13 JUNE      1996      UPDATE PRIMARY VARIABLES AFTER CONVERGENCE IS ACHIEVED
OUT      2.5      18 APRIL     1996      PRINT RESULTS FOR ELEMENTS, CONNECTIONS, AND SINKS/SOURCES
OBSERVED 2.4       4 AUGUST    1996      #78: RETURNS OBSERVED DATA AS A FUNCTION OF TIME
OBJFUN   2.5      21 MARCH     1996      #49: COMPUTE OBJECTIVE FUNCTION
WRITEPAR 1.0      17 JUNE      1996      #56: WRITE BEST FIT PARAMETER SET AND BLOCK ROCKS
PLOTFILE 3.2       6 OCTOBER   1997      #58: WRITES PLOTFILE IN PLOPO-FORMAT
JAC      3.1      24 FEBRUARY  1997      #51: CALCULATES FINITE DIFFERENCE JACOBIAN
MLLAMBDA 2.2      14 FEBRUARY  1994      #67: ESTIMATES NEW LAMBDAS
TERMINAT 3.2      13 MAY       1998      61: PERFORM ERROR ANALYSIS AND TERMINATE ITOUGH2
WRIFI    2.5      13 JANUARY   1996      AT THE COMPLETION OF A TOUGH2 RUN, WRITE PRIMARY VARIABLES ON FILE *SAVE*
QFISHER  2.2      16 FEBRUARY  1994      #77: RETURNS QUANTILE OF F-DISTRIBUTION
QCHI     1.0       1 AUGUST    1992      #88: RETURNS CHI-SQUARE QUANTILE
POLYNOM  1.0       1 AUGUST    1992      #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 DF6 R00*].

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.

```
?!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
ESTIMATED PARAMETER  V/L/F   ROCKS   PAR   INITIAL GUESS   BEST ESTIMATE              STANDARD DEVIATIONS          SENSITIVITY
                                                                              A PRIORI        JOINT       C/J     OUTPUT   OBJ. FUNC.
log(abs. perm.)      LOG10   SAND +1   1  -0.1200000E+02  -0.1169897E+02          N/A  0.8606E-02     0.514      608.3         0.952
POROSITY SAND        VALUE   SAND      1   0.2500000E+00   0.3500000E+00          N/A  0.8242E-02     0.455      222.4         0.872
Gas entrapped        VALUE   DEFAU     2   0.1025000E+02   0.1030000E+02          N/A  0.2315E-02     0.797      489.7         2.647
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

Figure 2.9.1. Excerpt from ITOUGH2 output file *vvRITi.v30.out*, showing inverse modeling results obtained with previously qualified version ITOUGH2 V3.0.

```
?!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
ESTIMATED PARAMETER  V/L/F   ROCKS   PAR  INITIAL GUESS    BEST ESTIMATE              STANDARD DEVIATIONS          SENSITIVITY
                                                                              A PRIORI        JOINT       C/J     OUTPUT   OBJ. FUNC.
log(abs. perm.)      LOG10   SAND +1   1    -0.12000E+02     -0.11699E+02          N/A   0.861E-02     0.514      608.3         0.952
POROSITY SAND        VALUE   SAND      1     0.25000E+00        0.350E+00          N/A   0.824E-02     0.455      222.4         0.872
Gas entrapped        VALUE   DEFAU     2     0.10250E+02      0.10300E+02          N/A   0.231E-02     0.797      489.7         2.647
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

Figure 2.9.2. Excerpt from ITOUGH2 output file *vvRITi.out*, showing inverse modeling results obtained with ITOUGH2 V3.2.

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	*vvFM1A* *vvFM1B*	*vvFM1A.out* *vvFM1B.out*	yes
1.2	Upstream saturation	*vvFM2A* *vvFM2B*	*vvFM2A.out* *vvFM2A.sav* *vvFM2B.ou*	yes
1.3	Upstream saturation times a constant	*vvFM3A* *vvFM3B*	*vvFM3A.out* *vvFM3A.sav* *vvFM3B.out*	yes
1.4	Upstream relative permeability	*vvFM4A* *vvFM4B*	*vvFM4A.out* *vvFM4B.ou*	yes
1.5	Upstream relative permeability times a factor	*vvFM5A* *vvFM5B*	*vvFM5A.out* *vvFM5B.ou*	yes
2	Free drainage boundary condition	*vvFDBC*	*vvFDBC.out*	yes
3	Active Fracture Concept	*vv*	*vv.out*	yes
4.1	Modification of Brooks-Corey capillary pressure function	*vvi* *vv*	*vvi_ch.tec*	yes
4.2	Modification of van Genuchten capillary pressure function	*vvi* *vv*	*vvi_ch.tec*	yes
5	New observation types SECONDARY and HEAT FLOW	*vv* *vvi*	*vvi.out* *vv.out*	yes
6	New priorities in porosity definition	*vvi* *vv*	*vv.out*	yes
7	Adjusting array dimensions	*vvRITi* *vvRIT* *vvRIT.dat* *minsize.inc*	*vvRITi.out*	yes
8	Application control	*vvRITi* *vvRIT* *vvRIT.dat*	*vvRITi.out*	yes
9	Regression testing	*vvRITi* *vvRIT* *vvRIT.dat*	*vvRITi.out* *vvRIT.v30.out*	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.

References

Finsterle, S., *ITOUGH2 Sample Problems*, Report LBNL-40042, Lawrence Berkeley National Laboratory, Berkeley, Calif., 1997.

Finsterle, S., *ITOUGH2 Command Reference, Version 3.2*, Report LBNL-40041 (updated), Lawrence Berkeley National Laboratory, Berkeley, Calif., 1998.

Finsterle, S., K. Pruess, and P. Fraser, *ITOUGH2 Software Qualification*, Report LBNL-39489, Lawrence Berkeley National Laboratory, Berkeley, Calif., 1997.

Liu, H. H., C. Doughty, and G. S. Bodvarsson, An active fracture model for unsaturated flow and transport in fractured rocks, *Water Resour. Res.*, (in press), 1998.

Luckner, L., M. Th. van Genuchten, and D. Nielsen, A consistent set of parametric models for the two-phase flow of immiscible fluids in the subsurface, *Water Resour. Res., 25*(10), 2187–2193, 1989.

Pruess, K., *TOUGH User's Guide*, Nuclear Regulatory Commission Report NUREG/CR-4645; also Report LBL-20700, Lawrence Berkeley Laboratory, Berkeley, Calif., 1987.

Pruess, K., *TOUGH2—A General Purpose Numerical Simulator for Multiphase Fluid and Heat Flow*, Report LBL-29400, Lawrence Berkeley Laboratory, Berkeley, Calif., 1991.

Pruess, K., A. Simmons, Y.-S. Wu, and G. Moridis, *TOUGH2 Software Qualification*, Report LBL-38383, Lawrence Berkeley National Laboratory, Berkeley, Calif., 1996.

Wu, Y.-S., C. F. Ahlers, P. Fraser, A. Simmons, and K. Pruess, *Software Qualification of Selected TOUGH2 Modules*, Report LBNL-39490, Lawrence Berkeley National Laboratory, Berkeley, Calif., 1996.

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 f1com.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 mdepcray.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 mdephp.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........


              @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
              @                                              @
              @  @@@  @@@@@   @@   @  @   @@@  @  @   @@@@   @
              @   @     @    @  @  @  @  @     @  @  @    @  @
              @   @     @    @  @  @  @  @ @@  @@@@     @@   @
              @   @     @    @  @  @  @  @  @  @  @    @@    @
              @  @@@    @     @@    @@    @@@  @  @  @@@@@@  @
              @                                              @
              @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


   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
+++++++++++++++

(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
++++++++++++++

(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
+++++++++

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
+++++++++++

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.

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


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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.......READ.ME..........READ.ME..........READ.ME..........READ.ME.......
```