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.

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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........

              @@@@
```

```
                    (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.....