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Modifications and Additions to Selected TOUGH2 Modules

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Earth Sciences Division

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1. Introduction

The purpose of this report is to provide all software baseline documents necessary for the software qualification of the revised versions of the selected TOUGH2 modules, which include single-phase gas (EOS1G), effective continuum method (EOS3/ECM), saturated/ unsaturated flow (EOS9), and radionuclide transport (T2R3D) modules of the TOUGH2 code. TOUGH2 is a numerical simulation code for multi-dimensional, coupled fluid and heat flow of multiphase, multicomponent fluid mixtures in porous and fractured media. This report augments the document Software Qualification of Selected TOUGH2 modules (Wu et al., 1996).

Wu and others (1996) have documented the software qualification of the original versions of the single-phase gas (EOS1G), effective continuum method (ECM), saturated/unsaturated flow (EOS9), and radionuclide transport (T2R3D) modules of TOUGH2. Subsequent to the software qualification reported in the above document, a number of additions and modifications have been carried out to these modules as requested by the Yucca Mountain project. In accordance with Yucca Mountain Project (YMP)/ Lawrence Berkeley National Laboratory (LBNL) Quality Implementing Procedure YMP-LBNL-QIP-SI.0, Software Qualification, all the changes are explicitly listed out along with the need/rationale for the modifications/additions.

This report contains the following sections: 1) Requirement specifications and code development and 2) Software validation test plan and results. These sections comprise sequential parts of Software Lifecycle, and should be used in conjunction with the TOUGH User's Guide (Pruess, 1987), TOUGH2 documentation (Pruess, 1991), TOUGH2 Software Qualification (Pruess et al., 1996), and Software Qualification of Selected TOUGH2 modules (Wu et al., 1996).

The version of TOUGH2 used with the software being qualified herein is the October 1996 Standard Version 1.2, as qualified in Wu et al. (1996) and housed at the Department of Energy's Energy Science and Technology Software Center (ESTSC) in Oak Ridge, Tennessee.

TOUGH2 and MULKOM

TOUGH2, a numerical simulator for non-isothermal flows of multicomponent, multi-phase fluids in porous and fractured media (Pruess, 1987,1991; Pruess et al. 1996), belongs to the MULKOM family of codes (Pruess, 1983, 1988) and is a more general version of the TOUGH simulator (Pruess, 1987). TOUGH2 is essentially a subset of

MULKOM, consisting of a selection of the better tested and documented MULKOM program modules. The MULKOM family of multi-phase, multi-component codes were developed at Lawrence Berkeley Laboratory primarily for geothermal reservoir applications (Pruess, 1983).

2. Requirements Specification

This section describes specific requirments for each addition to the various modules being qualified through this report, and should be considered in addition to those previously covered in Wu et al. (1996).

Single-Phase Gas Module (EOS1G)

The single-phase gas module differes from the previously qualified EOS1G module of TOUGH2 Version 1.2 in one way: implementation of a new relative peremeability function. Otherwise, all capabilities of the TOUGH2 code are preserved in this module.

Saturated/Unsatutaed Flow Module (EOS3/EOS9) and Transport Module (T2R3D)

The saturated/unsaturated flow modules (EOS3 and EOS9) and the transport module (T2R3D) differ from the previously qualified modules of TOUGH2 Version 1.2 in the following aspects: implementation of various interface area reduction schemes for fracture-matrix interaction in dual k media; modified weighting scheme for vitric/zeolitic interface; postprocessing of data for output of fluxes and velocities for visualization; input of spatially varying rock properties and capillary pressure modification at residual water saturation. Otherwise, all capabilities of the TOUGH2 code are preserved in this module.

2.1 Requirements

Various requirements regarding flow processes, physics, phase change and interaction, heat transport, dimensionality, geometry, grid generation, flexible specification of initial and boundary conditions, sources and sinks, automatic time-stepping, restart capability, internal version control and modularized structure for modifying and adding capabilities are the same as those specified in TOUGH2 Version 1.2.

Sample problems to illustrate code use and verify accuracy for the modifications listed above are discussed in the following sections.

2.2 Prior Examples of Requirement Verification

TOUGH2 has been verified and benchmarked by many fluid and heat flow problems that involved one, two, and three-dimensional flows, with varying degrees of non-linearity and coupling between heat and fluid flows, and different boundary conditions. These results substantiate the accuracy of the process description as well as the mathematical and numerical approaches used. See section 3 (Wu et al., 1996) for the design and description of the problems and section 4 (Wu et al., 1996) for the validation tests for the modules mentioned above.

3. Design Description

The formal structure and architecture of the different modules, functional requirements of the software and the implementation details are discussed in detail in Wu et al. (1996). Considerations of code design, structure, logic, data structure and flow, performance requirements and design constraints of the TOUGH2 code is given in Pruess et al. (1996).

3.1 Mathematical and Numerical Formulation

In terms of the integral formulation, the conservation equations of mass and thermal energy, solved by the standard TOUGH2 code, are described (Pruess, 1991) by

$$\frac{d}{dt}\int_{V_n} M^{(\kappa)}dV = \int_{\Gamma_n} \mathbf{F}^{(\kappa)} \bullet \mathbf{n}\, d\Gamma + \int_{V_n} q^{(\kappa)}dV \tag{1}$$

The integration here is over an arbitrary subdomain V_n of the flow system under study, which is bounded by the closed surface Γ_n. The quantity M appearing in the accumulation term denotes mass or energy per unit volume, with κ = 1(air) and κ = 2(water), labeling the mass components, and κ = 3 for "heat" component. $\mathbf{F}$ is a general "flow" term including multiphase Darcy's flow, mass advection/diffusion transport and heat convection/conduction transfer, $\mathbf{n}$ is an unit vector normal to the surface Γ and q is a sink/source term.

Based on the "integral finite difference" method (Edwards, 1972; Narasimhan and Witherspoon, 1976) the continuum equations are discretized in space using appropriate volume averages and surface integrals approximated as a discrete sum of averages over suraface segments A_{mn} [see Appenix B of Pruess(1991) for details]. Time is discretized as a first order backward difference which results in the following set of coupled non-linear, algebraic equations

$$R_n^{\kappa,k+1} = M_n^{\kappa,k+1} - M_n^{\kappa,k} - \frac{\Delta t}{V_n}\left[\sum_m A_{nm}F_{nm}^{\kappa,k+1} + V_n q_n^{\kappa,k+1}\right] = 0 \tag{2}$$

The component flux:

$$F_{nm}^{\kappa} = \sum_{\beta} X_{\beta}^{\kappa} F_{\beta,m} \tag{3}$$

where $X^{\kappa}{}_{\beta}$ is mass fraction of component κ in phase β. Individual phase mass fluxes, $F_{\beta,nm}$, are given by a multi-phase version of Darcy's law:

$$F_{\beta,nm} = -k_{nm}\left[\frac{k_{r\beta}\rho_{\beta}}{\mu_{\beta}}\right]_{nm}\left[\frac{P_{\beta,n} - P_{\beta,m}}{D_{nm}} - \rho_{\beta,nm}g_{nm}\right] \tag{4}$$

In Equation (4), k_{nm} is the absolute permeability, k_{rb} is relative permeability of phase b, m_b is viscosity of phase b, and P_b is the pressure in phase b. g_{nm} denotes a component of the vector of gravitational acceleration.

The entire geometric information of the space discretization in Equations (2) and (4) is provided through the grid block volumes V_n, interface area A_{mn}, nodal distances D_{mn} and components g_{mn} of gravitational acceleration along nodal lines. The subscript (nm) denotes

a suitable averaging at the interface between grid blocks n and m using the various weighting schemes.

3.2 Software and Hardware Considerations

The TOUGH2 code with the various modules (EOS3, EOS9, T2R3D) are portable to platforms that have an ANSI (FORTRAN 77) compiler. TOUGH2 can run on different platforms which include IBM Pcs, Macintosh, Unix workstation, or a mainframe.

3.3 Performance Requirements and Design Constraints

Changes made to address specific issues in each of the modules are listed as the following:

3.3.1 Interface area reduction scheme

For studying flow and transport in unsaturated fractured media, an important aspect is the evaluation of interaction between matrix blocks and the surrounding fractures. In the dual-permeability model, the fractured blocks interact with the matrix blocks according to the interface area between the two connecting blocks and their respective state variables. In the previous qualified version (Pruess et al., 1996), the complete fracture-matrix interface area was available by the setting isotropic parameter, ISOT=1, for each fracture-matrix connection. However, there is evidence that fracture-matrix interaction in the unsaturated zone at Yucca Mountain is limited due to fingering flow in fractures (Glass et al., 1996) and mineral coatings on the fracture surfaces, and in fact there may be only part of fracture-matrix interface areas that contributes fracture-matrix inter flow. Details of the conceptual models to reduce the fracture-matrix interface area have been proposed by Thoma et al. (1992), Altman et al. (1996), Ho (1997), and Bodvarsson et al. (1997).

In TOUGH2 the input data specified in CONNE introduces information for the connection between elements (Pruess, 1987). The format is as given below

Card CONNE.1
Format (A3,I2,A3,I2,4I5,4E10.4)
L1, NE1, EL2, NE2, NSEQ, NAD1,NAD2, ISOT, D1, D2,AREAX, BETAX

Specifically in CONNE.1, the parameter ISOT is set equal to 1, 2 or 3 which allows assignments of different anisotropic permeabilities for the materials in elements (EL1, NE1) and (EL2, NE2) making up the connection. AREAX is the interface area (m^2).

A number of reduction approaches for fracture/matrix interface areas have been implemented for use in the dual-permeability flow simulations of the UZ model. Different cases are treated in all the revised modules by setting ISOT to a proper negative value (-1, -3,-4,-7,-8,-9) which triggers different treatment for the reduction of the fracture-matrix interface area.These are discussed in detail in the section related to validation test plan and results.

3.3.2 Modified weighting scheme for vitric/zeolitic interface

The TOUGH2 code is presently used for modeling fluid and heat flow and chemical transport at the Yucca Mountain site. A major task in building the numerical model is an accurate representation of the complex geological layering and structure resulting from numerous periods of volcanism and tectonism since the Miocene. In the vertical direction,

4

heterogeneities primarily result from the deposition of ash flow and air fall tuffs found beneath Yucca Mountain. One major complexity is the post-depositional activity related to hydrothermal alteration. This is of special importance in the hydrologically significant vitric and zeolitic portions of the Calico Hills and Prow Pass formations, because permeabilities vary by several orders of magnitude when crossing the vitric/zeolitic interfaces in these units (Hinds et al., 1997; Bandarruga et al., 1997).

For the vertical vitric/zeolitic matrix-matrix interface, a modified downstream weighting scheme has been proposed and implemented into the TOUGH2 code. In this scheme, vertical downward matrix to matrix flow is evaluated using the mobility of the underlying, low-permeable zeolitic blocks in order to avoid over-estimates of flow into the zeolitic matrix blocks. It should be mentioned that in petroleum literature, upstream weighting is traditionally used for relative permeabilities and harmonic weighting is used for absolute permeabilities in handling multi-phase flow in porous media. This conventional technique works reasonably well for cases of multiphase flow as long as contrasts in flow properties of adjacent formation layers are not very large, such as in single porosity media. For simulating multiphase flow in fractured/porous media, Tsang and Pruess (1990) recognized that this traditional weighting scheme gives artificial flow resistance and can lead to physically incorrect solutions for highly heterogeneous composite formations with alternate layers of non-welded and welded tuffs, such as at Yucca Mountain. Therefore, except for the vitric/zeolitic matrix-matrix connections, full upstream weighting scheme is recommended to use for both relative and absolute permeabilities in order to obtain physically plausible solutions.

3.3.3 Post-processing for mass flux and flow velocity

A new subroutine for the calculation of the velocity and mass flux at each node is developed. This subroutine (vel_c) takes into account the irregular features of the grid and calculates the pore velocity and mass flux vectors using the state variables in the neighbouring elements at user's specified time steps. The objective of this subroutine is to speed up the post-processing in analyzing the TOUGH2 output, because neither pore velocity nor mass flux in the global coordinates is given in the standard TOUGH2 output.

The procedure for converting the local fluxes along connections in the local coordinates to a mass flux, F_n in the global coordinates (x, y, z) at the block center for block n of the grid is through the "projected area weighting method" (Wu et al., 1996). In this weighting scheme, the flux component, $F_{n,i}$ of the vector F_n is computed as the vectorial summation of the components of all local connection vectors in the same direction, weighted by the projected area in that direction,

$$F_{n,i} = \frac{\sum_m (A_{nm} \mid n_i \mid)(F_{nm} n_i)}{\sum_m (A_{nm} \mid n_i \mid)} \qquad (i = x, y, z) \tag{5}$$

where m is the total number of connections between element n and all its neighbouring elements m and F_{nm} is the flux along connection nm in the local coordinate system. n_i with i = x, y and z is the component in the x-,y-, and z-direction, respectively, of the unit vector **n** vector along the connection line nm between the two blocks n and m. In Equation (5), the term $[A_{nm} \mid n_i \mid]$ is the projected area of the interface A_{nm} on the direction i of the global coordinate system, and $(F_{nm} n_i)$ gives the flux component in the direction i of the global coordinate system contributed by the local flux F_{nm} between blocks n and m.

Similarly, a component, $v_{n,i}$, (i=x,y and z) of the pore velocity vector ($\mathbf{v}_n$) at a center of element block n is calculated by,

$$v_{n,i} = \frac{\sum_m (|n_i|)(v_{mn}n_i)}{\sum_m (|n_i|)} \qquad (i = x, y, z) \qquad (6)$$

Here a velocity component is weighted only by the interface area direction cosines.

3.3.4 Output files for visualization

The input data specified in block PARAM sets up the various computation parameters (Pruess, 1987). In particular in PARAM.1 a set of input parameters denoted by MOP(I), I=1, 24 are used. MOP(23) and MOP(24) are the two data fields that need to be specified to obtain the output files needed for visualization. The generation of the output is invoked by setting MOP(23) = 1 or 2. MOP(23)=0 does not lead to the post processing for flow velocity and flux calculations. Setting MOP(23)=1 leads to the various primary variables (pressure, temperature, liquid saturation, fracture saturation, and matrix saturation, capillary pressures and etc.) to be written to a file **tough2.tec** for non-dual permeability grids. For the dual permeability grids, **tough2.tec** is the output file for the matrix along with an additional file **tough_f.tec** for the fractures. MOP(23)=2 writes out the additional information about fluid velocities and mass fluxes besides the various primary variables listed above. MOP(24)=0 is a flag for non-dual permeability fields and MOP(24)=1 is for dual permeability simulations.

The output is written in a format suitable for prompt and easy visualization with standard commercial software used at LBNL. The post processing subroutine calculates the velocities and the mass fluxes in each of the three directions (x,y,z) for both the fracture and the matrix continuums. The nomenclature used in the output files for velocity and mass fluxes is as given below:

P   - Pressure, Pa
SL   - Liquid saturation
T   - Temperature, °C
Pcap – Capillary pressure, Pa
VLx - Liquid velocity in x direction, m/s
VLy - Liquid velocity in y direction, m/s
VLz - Liquid velocity in z direction, m/s
VFx - Liquid velocity in the fractures in x direction, m/s
VFy - Liquid velocity in the fractures in y direction, m/s
VFz - Liquid velocity in the fractures in z direction, m/s
VMx - Liquid velocity in the matrix in x direction, m/s
VMy - Liquid velocity in the matrix in y direction, m/s
VMz - Liquid velocity in the matrix in z direction, m/s
FFx - Mass flux in the fractures in x direction, $kg/s/m^2$
FFy - Mass flux in the fractures in y direction, $kg/s/m^2$
FFz - Mass flux in the fractures in z direction, $kg/s/m^2$
FMx - Mass flux in the matrix in x direction, $kg/s/m^2$
FMy - Mass flux in the matrix in y direction, $kg/s/m^2$
FMz - Mass flux in the matrix in z direction, $kg/s/m^2$
Ff-m - Mass flow rate between fractures and matrix, kg/s

3.3.5 Capillary pressure modification at residual water saturation

The standard TOUGH2 code allows for a selection of seven different capillary pressure versus water saturation functions (Pruess, 1987). In the case that van Genuchten's function (van Genuchten, 1980) is used, the capillary pressure increases very rapidly when liquid saturation is near residual water saturation. The theoretical limit at residual water saturation is infinity. Numerically the infinite pressure condition was avoided by imposing a finite, large value (such as 1.00E+11 Pa and higher) at the residual water saturation.

It has been observed, especially in modelling thermo-hydrological conditions in the unsaturated zone at Yucca Mountain, that heated rocks due to the thermal loading imposed on the system often lead to saturation conditions very near or even lower than residual saturations due to dry out of the matrix. However simulations of such drastic conditions were numerically very inefficient and unstable. It was very difficult to obtain numerical solutions due to numerical instability. This was of crucial concern in terms of computational times needed by the large number of simulations runs required for Total System Viability Assessment (TSVA) calculations for Yucca Mountain Project.

From a physical perspective, neither of the two conditions of infinite capillary pressure or a large cutoff value (discontinuity in derivative of the function) is correct. It was therefore decided to implement a linear interpolation scheme for capillary pressure at saturations near residual conditions. For a specified small value (e=1.0e-5 is the default), if the water saturation (S_w) decreases to less than S_{wir}+ e, the linear interpolation scheme is used to calculate the capillary pressure based on the slope of the straight line which is drawn tangent to the capillary pressure curve at a saturation of S_{wir} + e (Figure 1). This option is invoked only if ICP(1)=10, where ICP is the integer parameter to choose the type of capillary function specified in the input parameter set in ROCKS.1.3 of TOUGH2.
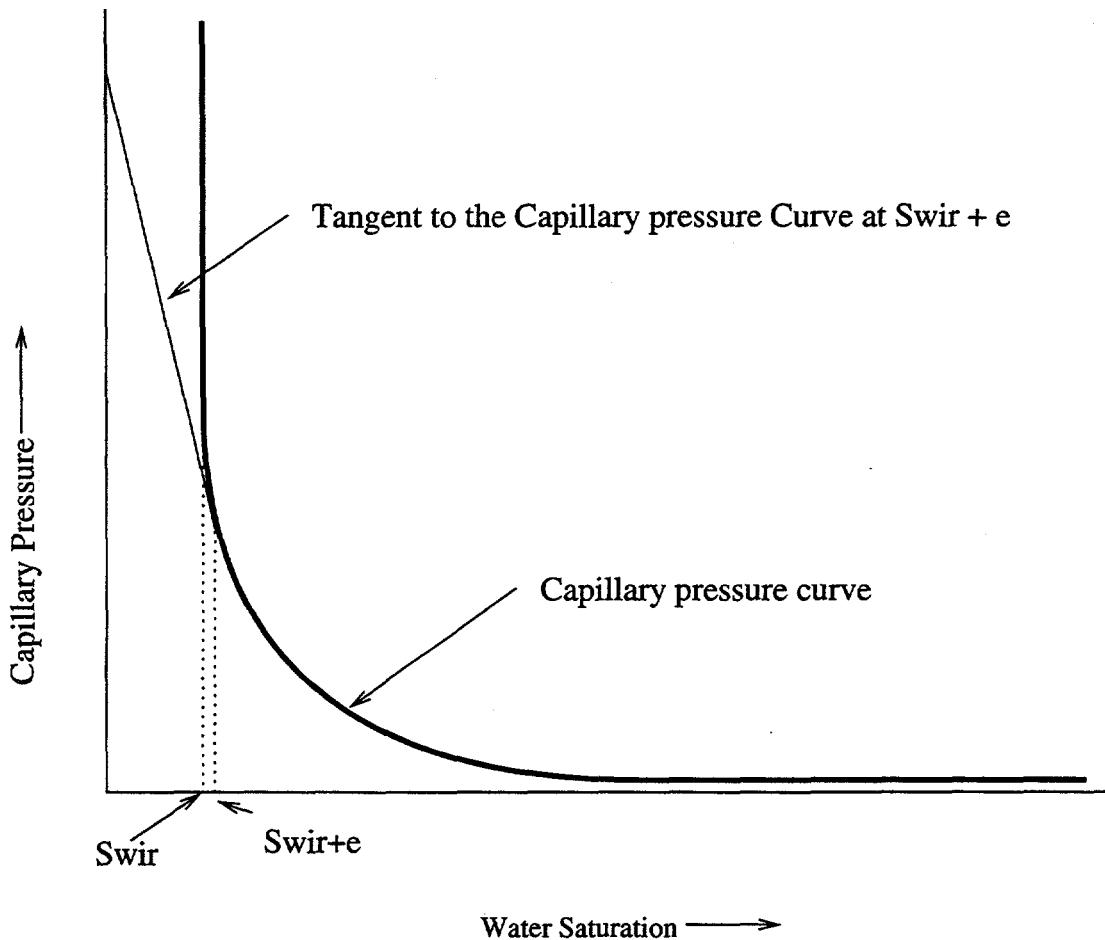
Figure 1. Schematic representation of the linear extrapolation scheme for capillary pressure at residual water saturation.

3.3.6 Data input for spatially varying rock properties

The rock properties for the various layers identified in the numerical model are input through the ROCKS.1 block in the input file. The implicit assumption using this format is that the various rock properties like permeability, porosity, grain density, thermal conductivity and rock grain specific heat are constant for a given rock type.

It is, however, common knowledge that most of these rock properties are heterogeneous. The spatial variability of a parameter is usually modeled using spatial random functions. Even though it is possible to input different material properties for each grid block using the qualified version of the TOUGH2 modules, computer storage and computational intensity become enormous when dealing with 3-D site-scale field problems. Therefore, special data input format for spatially varying rock properties and special treatment in the code are introduced here to improve the requirement of storage and computational intensity for large, spatially varying parameter cases. Various geostatistical techniques are available to generate the values of he parameter at each node from a set of measured values at various locations. The spatially varying case is used by the TOUGH2

code only when the keyword SVPAR is present in the input file. The method adopted in TOUGH2 is to set a flag (*isvpara =1* within t2fecm.f, t2f_9.f, or t2f2l2.f) and read an input file **svparam.dat** which reads the porosity, rock grain density and thermal conductivity for each element of the model. The default condition is *isvpara=0* in which case the rock properties from the input data set as specified in ROCKS is read in (Pruess, 1987).

3.3.7 Addition of a relative permeability function in EOS3/EOS9/T2R3D

The Brooks-Corey relative permeability function (Brooks and Corey, 1964) was added to the suite of other functions that are presently available in TOUGH2. This function has not been used in the UZ model to this date. In this formulation

$$k_{rl} = (S_l^*)^{\frac{2+3\lambda}{\lambda}} \tag{7}$$

$$k_{rg} = 1 - k_{rl} \tag{8}$$

$$\text{or } k_{rg} = (1 - S_l^*)^2 [1 - (S_l^*)^{\frac{2+\lambda}{\lambda}}] \tag{9}$$

$$\text{where } S_l^* = \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}} \tag{10}$$

$$\text{and } \lambda = \frac{m}{1 - m} \tag{11}$$

λ is a soil characteristic parameter and is related to m, the vanGenuchten parameter (van Genuchten, 1980), S_{lr} is the residual liquid saturation and S_{gr} is the residual gas saturation.

3.3.8 Addition of a relative permeability function in EOS1G

The qualified version of the TOUGH2 model is based on an explicit form of relative permeability to the liquid phase k_{rl} with the relative permeability to gas phase in the matrix, assumed to be $k_{rg}=1-k_{rl}$. However, the parameter of interest for the propagation of pneumatic signal through the unsaturated rocks is diffusivity, which is the ratio of the permeability to the air-filled porosity of a model layer. The primary pathway for gas is assumed to be through the fractures in the densely welded rock strata. The matrix porosity adjacent to fractures contributes little to gas flow but causes signal attenuation due to storage in the relatively large pore spaces. For the dual-permeability model with one matrix gridblock per layer, the $(1-k_{rl})$ formulation requires the estimated fracture permeability in the model to increase by several orders of magnitude in order to propagate the pneumatic signal down to the lower model layers (Bandurraga and Bodvarsson, 1997). The increases are not consistent with the air-k test results of LeCain (1997). Therefore, the Brooks-Corey type gas relative permeability model (Luckner et al., 1989) was instituted for the matrix to reduce k_{rg}. The new functional form of the relative permeability function gives rise to a larger interference of the gas phase. The new formulation provided a better match to the pneumatic test data.

The form of the equation is given by

$$S = \frac{S_l - S_{lr}}{S_{max} - S_{lr}} \qquad (12)$$

$$k_{rg} = (1-S)^2 \left[1 - S^{\frac{2+\lambda}{\lambda}} \right] \qquad (13)$$

$$\lambda = \frac{m}{1-m} \qquad (14)$$

where S_l is the liquid saturation, S_{lr} and S_{max} are the minimum and maximum liquid saturation (given as input in the ROCKS block as RP(2,mat) and RP(3,mat)) and m is the van Genuchten fitting parameter specified by RP(1,mat).

4. Software Validation Test Plan and Report

4.1 Validation Test Plan

The Validation Test Plan for the TOUGH2 modules consists of the TOUGH2 Validation Test Plan described in Pruess et al. (1996) and the verification test runs conducted to check the performance specifications listed above. Based on the Software Life Cycle approach, software verification refers to the checking procedure to ensure that implementation fulfils the requirements of the design stage, whereas validation means that the operational code satisfies all the provisions specified in the requirements stage.

4.1.1 Acceptance Criteria

Simulation results from the new modules should be in sufficient agreement with the numerical solutions using a validated code, and any differences should be less than one percent.

The acceptance criteria for these TOUGH2 modules are similar to those used for standard TOUGH2 (Pruess et., 1996; Wu et al., 1996). The acceptance criteria used in the previous studies (Wu et al., 1996) was the demonstartion that the results for the TOUGH2 simulation and the analytical solution differed by five percent or less (95% or better agreement). In this report, we have reduced the relative error to one percent since we are comparing results from numerical simulations only. The choice of one percent is arbitray but follows general conventions of numerical computations. The one percent error is defined as relative error, i.e. the difference between TOUGH2 and analytical solutions relative to the maximum changes in the concerned primary variables, such as pressure, saturation, mass fraction, and temperature.

4.2 Validation Tests

The validation tests for the revised modules consists of developing a sample problem set which addresses a specific issue (different interface area reduction scheme, for example) and using the qualified code and the revised code to check the output in each case for output variables. Very similar results (differences less than 1%) between the two versions of the codes would then lead to the conclusion that the revised code performs acceptably for qualification.

4.2.1 Sample problem 1:
Effective Continuum Method Module (ECM) using the EOS3 module

The sample problem considers one-dimensional (1-D) vertical flow in the unsaturated zone of Yucca Mountain and a single vertical column is extracted directly from the 3-D site scale model (Bodvarsson et al., 1997). The boundary condition specified is Dirichlet-type conditions. The bottom boundary is treated as being at constant gas pressure, liquid saturation, and temperature by specifying a large volume. A liquid water source is introduced to the second element from the top to provide constant water infiltration. See Figure 2 for the input file and Figure 3 for the output file. The results of simulations are presented in Table 1-4. Tables 1 and 2 compare the pressures in each element between the two versions of the code and show that the output is identical in both the cases. A similar conclusion is reached when the liquid fluxes are compared (Tables 3, 4).

```
ROCKS
tcw11      2 2480.     0.6200E-010.1600E-180.1600E-180.1600E-18 1.730        935.8
   1.0e-10                1.7300      0.2500           0.3626E-110.3626E-110.3626E-11
     11       0.2201    0.2000     0.1827    0.1000E-010.1000E+08          0.2900E-03
      9       0.2201    0.2000     0.1044E-040.1000E+130.1000E-010.1827    0.5187E-03
.
ptn21      2 2300.     0.4350     0.4000E-120.4000E-120.4000E-120.8500      1373.
   1.0e-10                0.8500
      7       0.2161    0.1000     1.000
      7       0.2161    0.1000     0.2536E-040.1000E+13 1.000


PARAM          123456789012345678901234
  4 20500     0500100000000000002030    140    0.00e-05
0.00000E003.15576E15 1.0000E04               dummy      -9.80665      3.0
1.0000e-5
0.900          00E+05             10.30           25.                      0.
TIMES
1    1
3.15576E16
RTSOL prec      rtol info iplvl nitmx nort kacc  iredb
       1.0e-6      0.1   0    1   250   15    2    0

     1.e-5      1.e15     100.0      100.     1.75      0.20      0.2    0

MULTI
2    3    2    8
START

ELEME
TP425          topbd0.2125E+050.0000E+00          0.1707E+060.2351E+060.1346E+04
11425          tcw110.1382E+060.0000E+00          0.1707E+060.2351E+060.1345E+04
12425          tcw120.1382E+060.0000E+00          0.1707E+060.2351E+060.1343E+04
13425          tcw130.6574E+050.0000E+00          0.1707E+060.2351E+060.1341E+04
.

65425          pp2zp0.8195E+060.0000E+00          0.1707E+060.2351E+060.7842E+03
71425          pp2zp0.6208E+060.0000E+00          0.1707E+060.2351E+060.7482E+03
BT425          botbd0.2125E+550.0000E+00          0.1707E+060.2351E+060.7316E+03

CONNE
11425TP425                   30.8800E+000.1000E-050.2125E+050.1000E+01
1242511425                   30.8800E+000.8800E+000.2125E+050.1000E+01
1342512425                   30.8800E+000.8800E+000.2125E+050.1000E+01
.
7142565425                   30.1668E+020.1924E+020.2125E+050.1000E+01
BT42571425                   30.1000E-050.1668E+020.2125E+050.1000E+01

GENER - Infiltration: 1.0 mm/yr, total water flow 0.67335839861079E-03 kg/s.
11425                          COM1 8.2136E-047.5610E+04
```

Figure 2. Input file for sample problem 1-D ECM formulation

```
INCON—INITIAL CONDITIONS FOR    26 ELEMENTS AT TIME   0.315576E+16
TP425             0.90000000E+00
0.8672450617412E+05 0.1099899979549E+02 0.1500000000000E+02
11425             0.62000000E-01
0.8673348582962E+05 0.1021823945263E+02 0.1502024658053E+02
12425             0.82000000E-01
0.8675144579527E+05 0.1010518548738E+02 0.1506024680222E+02


63425             0.33200000E+00
0.9152429077335E+05 0.1003940397232E+02 0.2757825199340E+02
64425             0.26600000E+00
0.9207478861318E+05 0.1002178172659E+02 0.2943272658169E+02
65425             0.28600000E+00
0.9246012069291E+05 0.1023457157415E+02 0.3058776266795E+02
71425             0.28600000E+00
0.9282690278093E+05 0.1023955879578E+02 0.3155102894970E+02
BT425             0.90000000E+00
0.9300000000000E+05 0.1000100000000E+02 0.3200000000000E+02

ENDCY
```

Figure 2. Input file for sample problem 1-D ECM formulation.

```
EOS3: EQUATION OF STATE FOR WATER-AIR MIXTURES
OPTIONS SELECTED ARE: (NK,NEQ,NPH,NB) = (2,3,2, 8)
                      NK  = 2    - NUMBER OF FLUID COMPONENTS
                      NEQ = 3    - NUMBER OF EQUATIONS PER GRID BLOCK
                      NPH = 2    - NUMBER OF PHASES THAT CAN BE PRESENT
                      NB  = 8    - NUMBER OF SECONDARY PARAMETERS (OTHER THAN
COMPONENT MASS FRACTIONS)

PHASE VOLUMES IN PLACE
GAS  0.74612E+06 M**3;    LIQUID  0.21358E+07 M**3
MASS IN PLACE
 GAS  0.77507E+06 KG;      LIQUID  0.21296E+10 KG;    AIR  0.79129E+06 KG;    VAPOR
0.13606E+05 KG;    LIQUID WATER  0.21295E+10 KG


 ...ITERATING...   AT [   1,   1] --- DELTEX = 0.100000E+05    MAX. RES. = 0.185359E-05
AT ELEMENT 53425   EQUATION   1
 61425(   1,  2) ST = 0.100000E+05 DT = 0.100000E+05 DX1= 0.444161E+00 DX2= -.204896E-
06 T =  25.539 P =     90915. S = 0.189791E-02
 .
 53425(  47,  2) ST = 0.315576E+16 DT = 0.113884E+16 DX1= -.749312E-11 DX2= 0.107294E-
14 T =  24.916 P =     90721. S = 0.427268E-01

    average inner-iteration/solve    =      1.0000000000000
         OUTPUT DATA AFTER (   47,   2)-2-TIME STEPS
THE TIME IS   0.36525E+11 DAYS

    TOTAL TIME     KCYC   ITER   ITERC   KON        DX1M         DX2M         DX3M
MAX. RES.        NER    KER        DELTEX
 0.31558E+16      47     2     104      2      0.91049E-11  0.45253E-14  0.23829E-12
0.41248E-05      20     2           0.11388E+16


 ELEM.  INDEX    P           T          SG        SL        XAIRG        XAIRL
PSAT        PCAP           Sf         Sm
             (PA)        (DEG-C)
(PA)        (PA)

 61425      1 0.90914E+05 0.25539E+02 0.16173E-02 0.99838E+00 0.97729E+00 0.14088E-04
0.32692E+04 -.22021E+06 0.99838E+00 0.99838E+00
 TP425      2 0.86723E+05 0.15000E+02 0.99900E+00 0.10002E-02 0.98768E+00 0.13666E-04
0.17039E+04 0.00000E+00 0.10002E-02 0.10002E-02
 11425      3 0.86732E+05 0.15020E+02 0.21824E+00 0.78176E+00 0.98766E+00 0.13668E-04
0.17061E+04 -.26035E+06 0.34051E+00 0.77165E+00
 12425      4 0.86750E+05 0.15060E+02 0.10519E+00 0.89481E+00 0.98763E+00 0.13670E-04
0.17105E+04 -.42420E+06 0.18449E+00 0.89599E+00
 .
 .
71425     25 0.92827E+05 0.31551E+02 0.23956E+00 0.76044E+00 0.96829E+00 0.14177E-04
0.46340E+04 -.13965E+07 0.52792E-01 0.74566E+00
BT425     26 0.93000E+05 0.32000E+02 0.10000E-02 0.99900E+00 0.96752E+00 0.14185E-04
0.47534E+04 -.14299E+07 0.99900E+00 0.99900E+00
```

Figure 3. Selected output for sample problem 1.

```
ELEM1   ELEM2   INDEX     FLOH        VEL(FRACT)      VEL(MATRX)      FLO(GAS)        FLO(LIQ.)
VEL(GAS)        VEL(LIQ.)     FLO(FRACT)    FLO(MATRX)
                             (W)                      (M/S)           (M/S)           (KG/S)
(KG/S)          (M/S)         (M/S)         (W)         (KG/S)          (KG/S)

        11425   TP425     1 -0.84579E+03   0.00000E+00   0.00000E+00   0.62591E-22
0.00000E+00   0.31485E-26   0.00000E+00   0.00000E+00   0.00000E+00
        12425   11425     2 -0.78368E+03   0.39141E-06   0.70523E-12  -0.11367E-07
0.82141E-03  -0.59601E-10   0.79815E-09   0.82069E-03   0.71640E-06
        .
        .
        71425   65425    24 -0.78368E+03   0.20202E-10   0.18061E-09  -0.12010E-07
0.82141E-03  -0.79230E-11   0.17736E-09   0.11993E-08   0.82141E-03
        BT425   71425    25 -0.78368E+03   0.17858E-09   0.17858E-09  -0.12036E-07
0.82141E-03  -0.60449E-09   0.17858E-09   0.82141E-03   0.82141E-03

   [KCYC,ITER] = [  47,   2]                                 THE TIME IS  0.31558E+16
SECONDS, OR  0.36525E+11 DAYS


PHASE VOLUMES IN PLACE
GAS   0.74608E+06 M**3;     LIQUID   0.21359E+07 M**3
MASS IN PLACE
GAS   0.77502E+06 KG;       LIQUID   0.21296E+10 KG;      AIR   0.79124E+06 KG;      VAPOR
0.13605E+05 KG;     LIQUID WATER   0.21296E+10 KG
```

Figure 3. Selected output for sample problem 1 (contd.).

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	8.67E+04	1.00E-03
11425	8.67E+04	7.82E-01
12425	8.68E+04	8.95E-01
63425	9.15E+04	9.61E-01
64425	9.21E+04	9.78E-01
65425	9.25E+04	7.65E-01
71425	9.28E+04	7.60E-01
BT425	9.30E+04	9.99E-01

Table 1. Steady-state pressure and liquid saturation profiles obtained using the modified version of the EOS3 module.

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	8.67E+04	1.00E-03
11425	8.67E+04	7.82E-01
12425	8.68E+04	8.95E-01
63425	9.15E+04	9.61E-01
64425	9.21E+04	9.78E-01
65425	9.25E+04	7.65E-01
71425	9.28E+04	7.60E-01
BT425	9.30E+04	9.99E-01

Table 2. Steady-state pressure and liquid saturation profiles obtained using the qualified version of the EOS3 module.

Eleme	Eleme	Liquid flow rate
		kg/s
12425	11425	8.21E-04
13425	12425	8.21E-04
63425	62425	8.21E-04
64425	63425	8.21E-04
65425	64425	8.21E-04
71425	65425	8.21E-04
BT425	71425	8.21E-04

Table 3. Steady-state mass flow rate in kg/s obtained using the modified version of the EOS3 module (ECM formulation).

Eleme	Eleme	Liquid flow rate
		kg/s
12425	11425	8.21E-04
13425	12425	8.21E-04
63425	62425	8.21E-04
64425	63425	8.21E-04
65425	64425	8.21E-04
71425	65425	8.21E-04
BT425	71425	8.21E-04

Table 4. Steady-state mass flow rate in kg/s obtained using the qualified version of the EOS3 module (ECM formulation).

4.2.2 Sample problem 2:
Input of spatially varying rock properties

Even though the qualified version of the EOS3/EOS9 modules has no restriction on the number of rock cards which assign heterogeneous parameters, practical applications of such approaches are limited due to requirement of computer storage and computational intensity for large field problems. Spatial variability of the different properties such as porosity and grain density is now being incorporated in the different conceptual models of flow and transport at Yucca Mountain. The inclusion of spatially variable rock properties in the TOUGH2 code is now facilitated through the use of **SVPAR** block in the input dataset (see Figure 4) and by needing an input file named **svparam.dat** for the porosity, grain density and specific heat of all the elements. The advantage of the additional data file is that the **svparam.dat** file could be generated thorugh the use of different geostatistical programs and the data file containing the spatial variability at different nodes could be directly read into the TOUGH2 code. Many other rock properties can be easily added to the input file if needed. An example of the svparam.dat is given in Table 5 and the output from the revised code and the qualified version is given in Tables 6 through 9 comparing the pressures and liquid saturations at steady-state conditions as well as liquid fluxes using the ECM EOS3 module.

```
PARAM             123456789012345678901234
4 20500      05001000000000002030     140      0.00e-05
0.00000E003.15576E15  1.0000E04               dummy       -9.80665      3.0
1.0000e-5
0.900           00E+05                10.30              25.                       0.

TIMES
1      1
3.15576E16
RTSOL prec        rtol  info iplvl nitmx nort kacc   iredb
     1.0e-6        0.1    0      1   250   15    2      0
        1.e-5      1.e15      100.0      100.      1.75       0.20        0.2    0

MULTI
2      3    2      8

START
GENER  - Infiltration: 1.0 mm/yr, total water flow 0.67335839861079E-03 kg/s.
11425                              COM1 8.2136E-047.5610E+04

INCON—INITIAL CONDITIONS FOR    26 ELEMENTS AT TIME   0.315576E+16
TP425               0.90000000E+00
0.8672450617412E+05  0.1099899979549E+02  0.1500000000000E+02
11425               0.62000000E-01
0.8673348582962E+05  0.1021823945263E+02  0.1502024658053E+02
BT425               0.90000000E+00
0.9300000000000E+05  0.1000100000000E+02  0.3200000000000E+02

SVPAR

ENDCY
```

Figure 4.   Input file for spatially varying parameters (sample problem 2).

Rock	Porosity	Density kg/m³	Sp.heat J/kg⁰C
topbd	0.9	2480	1.73
tcw11	6.20E-02	2480	1.73
tcw12	8.20E-02	2480	1.73
tsw35	0.13	2480	2.1
pp2zp	0.286	2300	1.56
pp2zp	0.286	2300	1.56
botbd	0.9	2300	1.56

Table 5. Example of the svparam.dat file where the porosity has been varied between the different rock types and/or model layers.

Eleme	Pressure Pa	Liq. Saturation
TP425	8.67E+04	1.0002E-03
11425	8.67E+04	7.8176E-01
12425	8.68E+04	8.9481E-01
13425	8.68E+04	8.7941E-01
63425	9.15E+04	9.6060E-01
64425	9.21E+04	9.7822E-01
65425	9.25E+04	7.6543E-01
71425	9.28E+04	7.6044E-01
BT425	9.30E+04	9.9900E-01

Table 6. Steady-state pressure and liquid saturation profiles obtained using the modified version of the EOS3 module where the spatially varying rock properties are input through the svparam.dat.

Eleme	Pressure Pa	Liq. Saturation
TP425	8.67E+04	1.0002E-03
11425	8.67E+04	7.8176E-01
12425	8.68E+04	8.9481E-01
13425	8.68E+04	8.7941E-01
63425	9.15E+04	9.6060E-01
64425	9.21E+04	9.7822E-01
65425	9.25E+04	7.6543E-01
71425	9.28E+04	7.6044E-01
BT425	9.30E+04	9.9900E-01

Table 7. Steady-state pressure and liquid saturation profiles obtained using the qualified version of the EOS3 module where the ROCKS block is used to input the varying porosities.

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Eleme	Eleme	Liquid Flow Rate
		kg/s
12425	11425	8.2141E-04
13425	12425	8.2141E-04
21425	13425	8.2141E-04
63425	62425	8.2141E-04
64425	63425	8.2141E-04
65425	64425	8.2141E-04
71425	65425	8.2141E-04
BT425	71425	8.2141E-04

Table 8. Steady-state mass flow rate in kg/s obtained using the modified version of the EOS3 module where svparam.dat is used to input the varying properties.

Eleme	Eleme	Liquid Flow Rate
		kg/s
12425	11425	8.2141E-04
13425	12425	8.2141E-04
21425	13425	8.2141E-04
63425	62425	8.2141E-04
64425	63425	8.2141E-04
65425	64425	8.2141E-04
71425	65425	8.2141E-04
BT425	71425	8.2141E-04

Table 9. Steady-state mass flow rate in kg/s obtained using the qualified version of the EOS3 module.

4.2.3 Dual permeability formulation with various interface area reduction factor

A series of sample problems using the various options for modifying the interface area between matrix and fracture is developed. The results are shown for EOS9 module but a identical procedure and subroutines are used for the EOS3 and T2R3D module too. The problem consists of a one-dimensional vertical grid with 45 non-uniform fracture and matrix elements, and 65 connections. This is a one-dimensional vertical moisture flow problem under two-phase and isothermal conditions. The bottom boundary element is set to constant liquid saturation by specifying a large volume. The second element from the top element is subjected to a constant water infiltration.

4.2.3.1 Sample problem 3: ISOT=-1

ISOT= -1 leads to reduction in the fracture-matrix interconnection area by the fraction of the upstream block liquid saturation in the dual-permeability model.

The methodology selected to compare the results between the revised code and the earlier version of the code is to obtain the steady-state condition using the revised version

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of the code by selecting the appropriate ISOT value (for example ISOT=-1 in Figure 5). This corresponds to the case of modifying the interface area by the upstream liquid saturation. From the results of the EOS9 module (Figure 6), the appropriate value of the liquid saturation in two blocks (Fj425/Mj425 and Fk425/Mk425) are selected based on the capillary pressure values in the fracture/matrix blocks. The interface area in the input file is accordingly modified. The interface area for the Fj425/Mj425 connection is reduced from 0.3491E+06 to 0.3729E+04 m^2 and the corresponding reduction for the connection Fk425/Mk425 is from 0.4769E+06 to 0.5129E+04 m^2 in the CONNE block in Figure 6. The qualified version of the code is then run with the input file as shown in Figure 7.

For the different cases considered here, we compare the pressure and the liquid saturation in the individual matrix and fracture elements (identified with M and F, respectively). Model elements are also labeled alphabetically with a lower case letter (Ma/Fa) starting from the surface. The element name also contains the map view element number. The input file for this problem is shown in Figure 5 and a section of the output file is given in Figure 6. The results are presented after 100 time steps (0.510221E+13 sec) in Tables 10 to 13. Also compared are the mass flow rates across different interfaces as shown below.

```
# input file
ROCKS
tcwM1     2 2480.      0.6600E-010.5400E-170.5400E-170.5400E-17 1.730        935.8
                         1.7300     0.2500
          7      0.2310    0.1300     1.000     0.2000E-01            0.5000E-03 5.086
          7      0.2310    0.1300     0.1150E-050.1000E+11 1.000
tcwM2     2 2480.      0.6600E-010.5400E-170.5400E-170.5400E-17 1.730        935.8
                         1.7300     0.2500
          7      0.2310    0.1300     1.000     0.2000E-01            0.5000E-03 5.086
          7      0.2310    0.1300     0.1150E-050.1000E+11 1.000
.
.
tcwF1     2 2480.      1.000     0.6030E-110.6030E-110.2290E-09 1.730        935.8
                         1.7300     0.2500                                   2.33E-4
          7      0.6330    0.1000E-01 1.000     0.2000E-01          · 0.5000E-03 5.086
          7      0.6330    0.1000E-010.2370E-020.1000E+11 1.000
tcwF2     2 2480.      1.000     0.6030E-110.6030E-110.1510E-09 1.730        935.8
                         1.7300     0.2500                                   2.99E-4
          7      0.6330    0.1000E-01 1.000     0.2000E-01            0.5000E-03 5.086
          7      0.6330    0.1000E-010.2370E-020.1000E+11 1.000
REFCO     0.920E+05      25.00

PARAM           12345678901234567890l234
 4 20100      01001000000000002030    1400    0.00e-05
0.00000E003.15576E181.0000E+01               dummy      -9.80665      3.0
1.0000e-3
0.800        00E+00            .920e5                25.                      0.
TIMES
1     1
3.15576E18

RTSOL prec      rtol info iplvl nitmx nort kacc  iredb
     1.0e-6      0.1   0   1  250   15    2    0
       1.e-5    1.e18    100.0     100.      1.30      0.20        0.2    1

START

GENER  base-case present day infiltration (flint et al) /3
Fa425                             COM1 0.4913E-080.7561E+05 0.000E+00
```

Figure 5. Input file for sample problem 3 - Dual-permeability EOS9, ISOT=-1.

```
ELEME
Fa425           tcwF10.8731E+050.1000E+01              172061.120234070.960 1228.3700
Ma425           tcwM10.3746E+050.0000E+00              172060.620234070.960 1228.3700
Fb425           tcwF20.1120E+060.1000E+01              172061.120234070.960 1221.4700
Mb425           tcwM20.3746E+050.0000E+00              172060.620234070.960 1221.4700
.
.
.
TP425           topbd0.4653E+040.0000E+00              172060.620234070.960 1231.8200
BT425           botbd0.4653E+540.0000E+00              172060.620234070.960  730.9700




CONNE
Fb425Fa425      0    0    0    30.3450E+010.3450E+010.4653E+040.1000E+01       1
Mb425Ma425      0    0    0    30.3450E+010.3450E+010.4653E+040.1000E+01       0
Fu425Ft425      0    0    0    30.2177E+020.2842E+020.4653E+040.1000E+01       1
Mu425Mt425      0    0    0    30.2177E+020.2842E+020.4653E+040.1000E+01       0
BT425Fu425      0    0    0    30.1000E-040.2177E+020.4653E+040.1000E+01       0
BT425Mu425      0    0    0    30.1000E-040.2177E+020.4653E+040.1000E+01       0
Fa425Ma425      0    0    0    10.0000E+000.1634E+000.7644E+050.0000E+00       2
Fb425Mb425      0    0    0    10.0000E+000.9107E-010.1371E+060.0000E+00       2
Fc425Mc425      0    0    0    10.0000E+000.1312E+000.7092E+050.0000E+00       2
Fi425Mi425      0    0    0    10.0000E+000.1515E+000.6336E+050.0000E+00       2
Fj425Mj425      0    0    0   -10.0000E+000.1650E+000.3491E+060.0000E+00       2
Fk425Mk425      0    0    0   -10.0000E+000.2415E+000.4769E+060.0000E+00       2
Fl425Ml425      0    0    0    10.0000E+000.8865E-010.6497E+060.0000E+00       2
Fm425Mm425      0    0    0    10.0000E+000.9208E-010.3649E+060.0000E+00       2

INCON

ENDCY
```

Figure 5. Input file for sample problem 3 - Dual-permeability EOS9, ISOT=-1 (contd.).

```
MESH HAS    44 ELEMENTS (    44 ACTIVE) AND    65 CONNECTIONS (INTERFACES) BETWEEN THEM
  GENER HAS    1 SINKS/SOURCES


  END OF TOUGH2 INPUT JOB --- ELAPSED TIME =    0.1101 SECONDS

EOS9: EQUATION OF STATE FOR SATURATED/UNSATURATED FLOW (RICHARDS EQUATION)
*

OPTIONS SELECTED ARE: (NK,NEQ,NPH,NB) = (1,1,1, 8)
                       NK  = 1   - NUMBER OF FLUID COMPONENTS
                       NEQ = 1   - NUMBER OF EQUATIONS PER GRID BLOCK
                       NPH = 1   - NUMBER OF PHASES THAT CAN BE PRESENT
                       NB  = 8   - NUMBER OF SECONDARY PARAMETERS (OTHER THAN
COMPONENT MASS FRACTIONS)

THE PRIMARY VARIABLE X1 IS PRESSURE FOR (X1.GE.0.920000E+05); IT IS LIQUID SATURATION
FOR (X1.LT. 1.)
...ITERATING...  AT [   1,  1] --- DELTEX = 0.100000E+02   MAX. RES. = 0.273094E-03
AT ELEMENT Fh425   EQUATION   1
 Fh425(   1,  2) ST = 0.100000E+02 DT = 0.100000E+02 DX1= -.456908E-04 DX2=
0.000000E+00 T =  25.000 P =        0. S = 0.167555E+00

 ++++++++ REDUCE TIME STEP AT ( 100,  5) +++++++++++++++++   NEW DELT = 0.476795E+12
 ...ITERATING...  AT [ 100,  1] --- DELTEX = 0.476795E+12   MAX. RES. = 0.222916E-01
AT ELEMENT Ft425   EQUATION   1
...ITERATING...  AT [ 100,  2] --- DELTEX = 0.476795E+12   MAX. RES. = 0.471528E+00
AT ELEMENT Mc425   EQUATION   1
 Mc425( 100,  3) ST = 0.510224E+13 DT = 0.476795E+12 DX1= -.863354E-03 DX2=
0.000000E+00 T =  25.000 P =        1. S = 0.965690E+00

    average inner-iteration/solve   =    0.98969072164948


          OUTPUT DATA AFTER ( 100,  3)-2-TIME STEPS
THE TIME IS  0.59054E+08 DAYS
```

Figure 6. Selected output for sample problem 3.

```
 TOTAL TIME     KCYC   ITER  ITERC   KON        DX1M          DX2M          DX3M
MAX. RES.       NER    KER        DELTEX
   0.51022E+13   100      3    294     2     0.62857E-02   0.00000E+00   0.00000E+00
0.20448E-03       6      1          0.47680E+12


 ELEM.  INDEX    PRES        S(liq)        PCAP        K(rel)       DIFFUS.         Sf
Sm
                  (PA)                      (PA)                    (m^2/s)
 Fa425      1  0.92000E+05  0.10593E-01  -.31177E+05  0.64319E-12  0.13287E-12  0.10593E-01
0.10593E-01
 Ma425      2  0.92000E+05  0.80380E+00  -.14951E+07  0.69084E-02  0.70064E-08  0.80380E+00
0.80380E+00. .
 Fu425     41  0.92000E+05  0.17675E-01  -.14679E+05  0.75701E-08  0.23674E-12  0.17675E-01
0.17675E-01
 Mu425     42  0.92000E+05  0.95990E+00  -.88501E+05  0.87971E-01  0.36368E-08  0.95990E+00
0.95990E+00
 TP425     43  0.92000E+05  0.10000E-01  0.00000E+00  0.00000E+00  0.00000E+00  0.10000E-01
0.10000E-01
 BT425     44  0.92000E+05  0.99000E+00  -.18654E+06  0.57642E+00  0.12588E-04  0.99000E+00
0.99000E+00


        ELEM1   ELEM2  INDEX    FLO(LIQ.)    VEL(LIQ.)    FLO(fract)    VEL(fract)
FLO(matrx)    VEL(matrx)
                                 (KG/S)       (M/S)        (KG/S)        (M/S)
(KG/S)        (M/S)
        Fb425   Fa425    1    0.71370E-08  0.62330E-09  0.71370E-08  0.62325E-09
0.00000E+00  0.00000E+00
        Mb425   Ma425    2    0.99857E-08  0.40582E-13  0.99857E-08  0.40569E-13
0.99857E-08  0.40569E-13
        Fa425   Ma425   45   -0.26636E-11 -0.32991E-17  0.00000E+00  0.00000E+00 -
0.26636E-11 -0.32991E-17
        Fb425   Mb425   46   -0.16644E-10 -0.11358E-16  0.00000E+00  0.00000E+00 -
0.16644E-10 -0.11358E-16
        Fc425   Mc425   47   -0.99293E-09 -0.12095E-14  0.00000E+00  0.00000E+00 -
0.99293E-09 -0.12095E-14
        Fq425   Mq425   61   -0.36168E-06 -0.51724E-13  0.00000E+00  0.00000E+00 -
0.36168E-06 -0.51724E-13
        Fr425   Mr425   62   -0.20029E-07 -0.37321E-14  0.00000E+00  0.00000E+00 -
0.20029E-07 -0.37321E-14
        Fs425   Ms425   63   -0.47430E-09 -0.31525E-14  0.00000E+00  0.00000E+00 -
0.47430E-09 -0.31525E-14
```

Figure 6. Selected output for sample problem 3 (contd.).

```
CONNE
Fb425Fa425     0    0    0    30.3450E+010.3450E+010.4653E+040.1000E+01      1
Mb425Ma425     0    0    0    30.3450E+010.3450E+010.4653E+040.1000E+01      0
Fa425TP425     0    0    0    30.3450E+010.1000E-040.4653E+040.1000E+01      0
Ma425TP425     0    0    0    30.3450E+010.1000E-040.4653E+040.1000E+01      0
Fu425Ft425     0    0    0    30.2177E+020.2842E+020.4653E+040.1000E+01      1
Mu425Mt425     0    0    0    30.2177E+020.2842E+020.4653E+040.1000E+01      0
BT425Fu425     0    0    0    30.1000E-040.2177E+020.4653E+040.1000E+01      0
BT425Mu425     0    0    0    30.1000E-040.2177E+020.4653E+040.1000E+01      0
Fa425Ma425     0    0    0    +10.0000E+000.1634E+000.7644E+050.0000E+00      2
Fb425Mb425     0    0    0    +10.0000E+000.9107E-010.1371E+060.0000E+00      2
Fj425Mj425     0    0    0    +10.0000E+000.1650E+000.3729E+040.0000E+00      2
Fk425Mk425     0    0    0    +10.0000E+000.2415E+000.5129E+040.0000E+00      2
Fl425Ml425     0    0    0    +10.0000E+000.8865E-010.6497E+060.0000E+00      2
Fm425Mm425     0    0    0    +10.0000E+000.9208E-010.3649E+060.0000E+00      2
Fs425Ms425     0    0    0    +10.0000E+000.2488E+010.8175E+040.0000E+00      2
Ft425Mt425     0    0    0    +10.0000E+000.2488E+010.3539E+050.0000E+00      2
Fu425Mu425     0    0    0    +10.0000E+000.2488E+010.2697E+050.0000E+00      2

INCON
Fa425               0.10000000E+01
0.2155949292959E-01 0.9000000000000E+05  0.2155949292959E-01  0.2155949292959E-01
TP425               0.20000000E+00
0.1000000000000E-01 0.8500000000000E+05  0.1000000000000E-01  0.1000000000000E-01
BT425               0.28000000E+00
0.9900000000000E+00 0.9199053658275E+05  0.9900000000000E+00  0.9900000000000E+00
ENDCY
```

Figure 7. Selected input to the qualified version of EOS9 for sample problem 3.

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0593E-02
Ma425	9.20E+04	8.0380E-01
Fi425	9.20E+04	1.0271E-02
Mi425	9.20E+04	7.7399E-01
Fj425	9.20E+04	1.0681E-02
Mj425	9.20E+04	4.6075E-01
Fk425	9.20E+04	1.0755E-02
Mk425	9.20E+04	5.9422E-01
Fl425	9.20E+04	1.1531E-02
Ml425	9.20E+04	8.3896E-01
Fm425	9.20E+04	1.2944E-02
Mm425	9.20E+04	6.8779E-01
BT425	9.20E+04	9.9000E-01

Table 10. Pressure and liquid saturation profiles obtained using the modified version of the EOS9 module after 100 timesteps (ISOT=-1).

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0593E-02
Ma425	9.20E+04	8.0380E-01
Fi425	9.20E+04	1.0271E-02
Mi425	9.20E+04	7.7399E-01
Fj425	9.20E+04	1.0681E-02
Mj425	9.20E+04	4.6075E-01
Fk425	9.20E+04	1.0755E-02
Mk425	9.20E+04	5.9422E-01
Fl425	9.20E+04	1.1531E-02
Ml425	9.20E+04	8.3896E-01
Fm425	9.20E+04	1.2944E-02
Mm425	9.20E+04	6.8779E-01
BT425	9.20E+04	9.9000E-01

Table 11. Pressure and liquid saturation profiles obtained using the qualified version of the EOS9 module after 100 timesteps (ISOT=-1).

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	7.1370E-09
Mb425	Ma425	9.9857E-09
Fi425	Fh425	3.5477E-15
Mi425	Mh425	4.4578E-07
Fj425	Fi425	5.7607E-10
Mj425	Mi425	4.5473E-07
Fk425	Fj425	1.3434E-08
Mk425	Mj425	7.2127E-07
Fl425	Fk425	3.6757E-08
Ml425	Mk425	1.3346E-06
Fm425	Fl425	6.3383E-08
Mm425	Ml425	1.4908E-06
Fi425	Mi425	-8.9539E-13
Fj425	Mj425	-2.3578E-12
Fk425	Mk425	-5.4393E-13
Fl425	Ml425	-1.0201E-09
Fm425	Mm425	-2.9863E-08

Table 12. Liquid flow rate in kg/s obtained using the modified version of the EOS9 module after 100 timesteps (ISOT=-1).

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.71371E-08
Mb425	Ma425	0.99852E-08
Fi425	Fh425	0.35472E-14
Mi425	Mh425	0.44576E-06
Fj425	Fi425	0.57608E-09
Mj425	Mi425	0.45471E-06
Fk425	Fj425	0.13434E-07
Mk425	Mj425	0.72123E-06
Fl425	Fk425	0.36758E-07
Ml425	Mk425	0.13345E-05
Fm425	Fl425	0.63383E-07
Mm425	Ml425	0.14907E-05
Fi425	Mi425	-0.89542E-12
Fj425	Mj425	-0.23580E-11
Fk425	Mk425	-5.43960E-13
Fl425	Ml425	-1.02010E-09
Fm425	Mm425	-2.98640E-08

Table 13. Liquid flow rate in kg/s obtained using the qualified version of the EOS9 module after 100 timesteps (ISOT=-1).

4.2.3.2 Sample problem 4: ISOT=-3

The reduction factor is the product of upstream relative permeability times a constant factor. The constant factor is input in the field RP(7) for each rock type of fractures where RP(I), I=1,7 are the various input data for relative permeability function given in the card ROCKS.1.2 (see Pruess, 1987 for details of input formats). The results are reported after a total time of 0.510224E+13 seconds in Tables 14 to 17.

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0593E-02
Ma425	9.20E+04	8.0379E-01
Fi425	9.20E+04	1.0271E-02
Mi425	9.20E+04	7.7399E-01
Fj425	9.20E+04	1.0681E-02
Mj425	9.20E+04	4.6074E-01
Fk425	9.20E+04	1.0755E-02
Mk425	9.20E+04	5.9422E-01
Fl425	9.20E+04	1.1531E-02
Ml425	9.20E+04	8.3896E-01
Fm425	9.20E+04	1.2944E-02
Mm425	9.20E+04	6.8779E-01
BT425	9.20E+04	9.9000E-01

Table 14. Pressure and liquid saturation profiles obtained using the modified version of the EOS9 module after 100 timesteps (ISOT=-3).

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0593E-02
Ma425	9.20E+04	8.0379E-01
Fi425	9.20E+04	1.0271E-02
Mi425	9.20E+04	7.7399E-01
Fj425	9.20E+04	1.0681E-02
Mj425	9.20E+04	4.6074E-01
Fk425	9.20E+04	1.0755E-02
Mk425	9.20E+04	5.9422E-01
Fl425	9.20E+04	1.1531E-02
Ml425	9.20E+04	8.3896E-01
Fm425	9.20E+04	1.2944E-02
Mm425	9.20E+04	6.8779E-01
BT425	9.20E+04	9.9000E-01

Table 15. Pressure and liquid saturation profiles obtained using the qualified version of the EOS9 module after 100 timesteps (ISOT=-3).

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.71370E-08
Mb425	Ma425	0.99849E-08
Fi425	Fh425	0.35468E-14
Mi425	Mh425	0.44574E-06
Fj425	Fi425	0.57607E-09
Mj425	Mi425	0.45469E-06
Fk425	Fj425	0.13437E-07
Mk425	Mj425	0.72119E-06
Fl425	Fk425	0.36761E-07
Ml425	Mk425	0.13345E-05
Fi425	Mi425	-0.89543E-12
Fj425	Mj425	-0.12036E-20
Fk425	Mk425	-0.40125E-21
Fl425	Ml425	-0.10202E-08

Table 16. Liquid flow rate in kg/s obtained using the modified version of the EOS9 module after 0.510224E+13 sec (ISOT=-3).

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.71370E-08
Mb425	Ma425	0.99849E-08
Fi425	Fh425	0.35468E-14
Mi425	Mh425	0.44574E-06
Fj425	Fi425	0.57607E-09
Mj425	Mi425	0.45469E-06
Fk425	Fj425	0.13437E-07
Mk425	Mj425	0.72119E-06
Fl425	Fk425	0.36761E-07
Ml425	Mk425	0.13345E-05
Fi425	Mi425	-0.89543E-12
Fj425	Mj425	-0.12036E-20
Fk425	Mk425	-0.40125E-21
Fl425	Ml425	-0.10202E-08

Table 17. Liquid flow rate in kg/s obtained using the qualified version of the EOS9 module after 0.510224E+13 sec (ISOT=-3).

4.2.3.3 Sample problem 5: ISOT=-4

For ISOT =-4, the reduction factor equal to relative permeability to liquid of the upstream block in the fracture-matrix dual-permeability connection as outlined by Ho (1997). The steady-state results for the 1-D column are presented in Tables 18 to 21.

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	2.2280E-02
Ma425	9.20E+04	9.4198E-01
Fi425	9.20E+04	1.0550E-02
Mi425	9.20E+04	9.8191E-01
Fj425	9.20E+04	1.1722E-02
Mj425	9.20E+04	9.1104E-01
Fk425	9.20E+04	1.7061E-02
Mk425	9.20E+04	9.9376E-01
Fl425	9.20E+04	2.5333E-02
Ml425	9.20E+04	9.9949E-01
Fm425	9.20E+04	3.4990E-02
Mm425	9.20E+04	9.7740E-01
BT425	9.20E+04	9.9000E-01

Table 18. Steady-state pressure and liquid saturation profiles obtained using the modified version of the EOS9 module   (ISOT=-4).

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	2.2280E-02
Ma425	9.20E+04	9.4198E-01
Fi425	9.20E+04	1.0550E-02
Mi425	9.20E+04	9.8191E-01
Fj425	9.20E+04	1.1722E-02
Mj425	9.20E+04	9.1104E-01
Fk425	9.20E+04	1.7061E-02
Mk425	9.20E+04	9.9376E-01
Fl425	9.20E+04	2.5333E-02
Ml425	9.20E+04	9.9949E-01
Fm425	9.20E+04	3.4990E-02
Mm425	9.20E+04	9.7740E-01
BT425	9.20E+04	9.9000E-01

Table 19. Steady-state pressure and liquid saturation profiles obtained using the qualified version of the EOS9 module   (ISOT=-4).

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.49125E-03
Mb425	Ma425	0.45572E-07
Fi425	Fh425	0.39063E-11
Mi425	Mh425	0.49130E-03
Fj425	Fi425	0.79352E-08
Mj425	Mi425	0.49129E-03
Fk425	Fj425	0.39500E-06
Mk425	Mj425	0.49090E-03
Fl425	Fk425	0.13028E-03
Ml425	Mk425	0.36102E-03
Fm425	Fl425	0.30854E-03
Mm425	Ml425	0.18276E-03
Fi425	Mi425	0.79313E-08
Fj425	Mj425	0.38707E-06
Fk425	Mk425	1.29880E-04
Fl425	Ml425	1.78260E-04
Fm425	Mm425	-3.6355E-06

Table 20. Steady-state liquid flow rate in kg/s obtained using the modified version of the EOS9 module (ISOT=-4).

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.49125E-03
Mb425	Ma425	0.45572E-07
Fi425	Fh425	0.39063E-11
Mi425	Mh425	0.49130E-03
Fj425	Fi425	0.79352E-08
Mj425	Mi425	0.49129E-03
Fk425	Fj425	0.39500E-06
Mk425	Mj425	0.49090E-03
Fl425	Fk425	0.13028E-03
Ml425	Mk425	0.36102E-03
Fm425	Fl425	0.30854E-03
Mm425	Ml425	0.18276E-03
Fi425	Mi425	0.79313E-08
Fj425	Mj425	0.38707E-06
Fk425	Mk425	1.29880E-04
Fl425	Ml425	1.78260E-04
Fm425	Mm425	-3.6355E-06

Table 21. Steady-state liquid flow rate in kg/s obtained using the qualified version of the EOS9 module (ISOT=-4).

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4.2.3.4 Sample problem 6: ISOT=-7

For ISOT=-7; the reduction factor for the fracture-matrix interface area is the normalized mass flux (f_m) through fractures given by the following relation $f_m = q_f/ q_{1-d}$ where q_f is the maximum mass flux through the fractures, defined as fracture mass flux under unit vertical hydraulic gradient, and q_{1-d} is a normalized factor, input by the user. The results are reported after a total time of 0.510224E+13 seconds in Tables 22 to 25.

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0593E-02
Ma425	9.20E+04	8.0379E-01
Fi425	9.20E+04	1.0271E-02
Mi425	9.20E+04	7.7399E-01
Fj425	9.20E+04	1.0681E-02
Mj425	9.20E+04	4.6074E-01
Fk425	9.20E+04	1.0755E-02
Mk425	9.20E+04	5.9422E-01
Fl425	9.20E+04	1.1531E-02
Ml425	9.20E+04	8.3896E-01
Fm425	9.20E+04	1.2944E-02
Mm425	9.20E+04	6.8779E-01
BT425	9.20E+04	9.9000E-01

Table 22. Pressure and liquid saturation profiles obtained using the modified version of the EOS9 module after 100 timesteps (ISOT=-7).

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0593E-02
Ma425	9.20E+04	8.0379E-01
Fi425	9.20E+04	1.0271E-02
Mi425	9.20E+04	7.7399E-01
Fj425	9.20E+04	1.0681E-02
Mj425	9.20E+04	4.6074E-01
Fk425	9.20E+04	1.0755E-02
Mk425	9.20E+04	5.9422E-01
Fl425	9.20E+04	1.1531E-02
Ml425	9.20E+04	8.3896E-01
Fm425	9.20E+04	1.2944E-02
Mm425	9.20E+04	6.8779E-01
BT425	9.20E+04	9.9000E-01

Table 23. Pressure and liquid saturation profiles obtained using the qualified version of the EOS9 module after 100 timesteps (ISOT=-7)

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.71370E-08
Mb425	Ma425	0.99849E-08
Fi425	Fh425	0.35468E-14
Mi425	Mh425	0.44574E-06
Fj425	Fi425	0.57607E-09
Mj425	Mi425	0.45469E-06
Fk425	Fj425	0.13437E-07
Mk425	Mj425	0.72119E-06
Fi425	Mi425	-0.89543E-12
Fj425	Mj425	-0.66769E-19
Fk425	Mk425	-0.40516E-19
Fl425	Ml425	-0.10202E-08
Fm425	Mm425	-0.29865E-07

Table 24. Liquid flow rate in kg/s obtained using the modified version of the EOS9 module after 100 timesteps (ISOT=-7).

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.71370E-08
Mb425	Ma425	0.99849E-08
Fi425	Fh425	0.35468E-14
Mi425	Mh425	0.44574E-06
Fj425	Fi425	0.57607E-09
Mj425	Mi425	0.45469E-06
Fk425	Fj425	0.13437E-07
Mk425	Mj425	0.72119E-06
Fi425	Mi425	-0.89543E-12
Fj425	Mj425	-0.66788E-19
Fk425	Mk425	-0.40518E-19
Fl425	Ml425	-0.10202E-08
Fm425	Mm425	-0.29865E-07

Table 25. Liquid flow rate in kg/s obtained using the qualified version of the EOS9 module after 100 timesteps (ISOT=-7).

4.2.3.5 Sample problem 7: ISOT=-8

For ISOT=-8, the reduction factor is the product of the normalized mass flux through fracture as calculated for ISOT=-7 times upstream liquid saturation of fracture and matrix blocks. The results for the modified version of the code and the earlier version are presented in Tables 26 to 29.

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0593E-02
Ma425	9.20E+04	8.0379E-01
Fi425	9.20E+04	1.0271E-02
Mi425	9.20E+04	7.7399E-01
Fj425	9.20E+04	1.0681E-02
Mj425	9.20E+04	4.6074E-01
Fk425	9.20E+04	1.0755E-02
Mk425	9.20E+04	5.9422E-01
Fl425	9.20E+04	1.1531E-02
Ml425	9.20E+04	8.3896E-01
Fm425	9.20E+04	1.2944E-02
Mm425	9.20E+04	6.8779E-01
BT425	9.20E+04	9.9000E-01

Table 26. Pressure and liquid saturation profiles obtained using the modified version of the EOS9 module after 100 timesteps (ISOT=-8).

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0593E-02
Ma425	9.20E+04	8.0379E-01
Fi425	9.20E+04	1.0271E-02
Mi425	9.20E+04	7.7399E-01
Fj425	9.20E+04	1.0681E-02
Mj425	9.20E+04	4.6074E-01
Fk425	9.20E+04	1.0755E-02
Mk425	9.20E+04	5.9422E-01
Fl425	9.20E+04	1.1531E-02
Ml425	9.20E+04	8.3896E-01
Fm425	9.20E+04	1.2944E-02
Mm425	9.20E+04	6.8779E-01
BT425	9.20E+04	9.9000E-01

Table 27. Pressure and liquid saturation profiles obtained using the qualified version of the EOS9 module after 100 timesteps (ISOT=-8).

Eleme	Eleme	Liquid flow rate kg/s
Fb425	Fa425	0.71370E-08
Mb425	Ma425	0.99849E-08
Fi425	Fh425	0.35468E-14
Mi425	Mh425	0.44574E-06
Fj425	Fi425	0.57607E-09
Mj425	Mi425	0.45469E-06
Fk425	Fj425	0.13437E-07
Mk425	Mj425	0.72119E-06
Fl425	Fk425	0.36761E-07
Ml425	Mk425	0.13345E-05
Fm425	Fl425	0.63386E-07
Mm425	Ml425	0.14906E-05
Fi425	Mi425	-0.89543E-12
Fj425	Mj425	-0.71318E-21
Fk425	Mk425	-4.35740E-22
Fl425	Ml425	-1.02020E-09
Fm425	Mm425	-2.98650E-08
Fn425	Mn425	-5.28350E-08

Table 28. Liquid flow rate in kg/s obtained using the modified version of the EOS9 module after 100 timesteps (ISOT=-8).

Eleme	Eleme	Liquid flow rate kg/s
Fb425	Fa425	0.71370E-08
Mb425	Ma425	0.99849E-08
Fi425	Fh425	0.35468E-14
Mi425	Mh425	0.44574E-06
Fj425	Fi425	0.57607E-09
Mj425	Mi425	0.45469E-06
Fk425	Fj425	0.13437E-07
Mk425	Mj425	0.72119E-06
Fl425	Fk425	0.36761E-07
Ml425	Mk425	0.13345E-05
Fm425	Fl425	0.63386E-07
Mm425	Ml425	0.14906E-05
Fi425	Mi425	-0.89543E-12
Fj425	Mj425	-7.1342E-22
Fk425	Mk425	-4.3572E-22
Fl425	Ml425	-1.02020E-09
Fm425	Mm425	-2.98650E-08
Fn425	Mn425	-5.28350E-08

Table 29. Liquid flow rate in kg/s obtained using the qualified version of the EOS9 module after 100 timesteps (ISOT=-8).

4.2.3.6 Sample problem 8: ISOT=-9

For ISOT=-9; reduction factor is a constant number (Altman et al., 1996). The constant factor is specified as RP(6) for each rock type in the input file and is in general obtained as an inversion parameter from ITOUGH2 (Bandurraga and Bodvarsson, 1997) based on the calibration of the 1-d model for water saturation, water potential and temperature data measured in the field.

The results are presented in Tables 30 to 33.

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0593E-02
Ma425	9.20E+04	8.0379E-01
Fi425	9.20E+04	1.0271E-02
Mi425	9.20E+04	7.7399E-01
Fj425	9.20E+04	1.0681E-02
Mj425	9.20E+04	4.6075E-01
Fk425	9.20E+04	1.0755E-02
Mk425	9.20E+04	5.9422E-01
BT425	9.20E+04	9.9000E-01

Table 30. Pressure and liquid saturation profiles obtained using the modified version of the EOS9 module after 100 timesteps (ISOT=-9).

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0593E-02
Ma425	9.20E+04	8.0379E-01
Fi425	9.20E+04	1.0271E-02
Mi425	9.20E+04	7.7399E-01
Fj425	9.20E+04	1.0681E-02
Mj425	9.20E+04	4.6075E-01
Fk425	9.20E+04	1.0755E-02
Mk425	9.20E+04	5.9422E-01
BT425	9.20E+04	9.9000E-01

Table 31. Pressure and liquid saturation profiles obtained using the qualified version of the EOS9 module after 100 timesteps (ISOT=-9).

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.71370E-08
Mb425	Ma425	0.99850E-08
Fi425	Fh425	0.35468E-14
Mi425	Mh425	0.44574E-06
Fj425	Fi425	0.57607E-09
Mj425	Mi425	0.45469E-06
Fk425	Fj425	0.13436E-07
Mk425	Mj425	0.72119E-06
Fl425	Fk425	0.36761E-07
Ml425	Mk425	0.13345E-05
Fm425	Fl425	0.63386E-07
Mm425	Ml425	0.14906E-05
Fi425	Mi425	-0.89543E-12
Fj425	Mj425	-0.11039E-12
Fk425	Mk425	-2.52920E-14
Fl425	Ml425	-1.02020E-09
Fm425	Mm425	-2.98650E-08

Table 32. Liquid flow rate in kg/s obtained using the modified version of the EOS9 module after 100 timesteps (ISOT=-9).

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.71370E-08
Mb425	Ma425	0.99850E-08
Fi425	Fh425	0.35468E-14
Mi425	Mh425	0.44574E-06
Fj425	Fi425	0.57607E-09
Mj425	Mi425	0.45469E-06
Fk425	Fj425	0.13436E-07
Mk425	Mj425	0.72119E-06
Fl425	Fk425	0.36761E-07
Ml425	Mk425	0.13345E-05
Fm425	Fl425	0.63386E-07
Mm425	Ml425	0.14906E-05
Fi425	Mi425	-0.89543E-12
Fj425	Mj425	-0.11043E-12
Fk425	Mk425	-2.52970E-14
Fl425	Ml425	-1.02020E-09
Fm425	Mm425	-2.98650E-08

Table 33. Liquid flow rate in kg/s obtained using the qualified version of the EOS9 module after 100 time steps (ISOT=-9).

4.2.4 Sample problem 9:

Modified weighting scheme for vitric/zeolitic matrix interface

A one-dimensional column as described for the earlier problems is used. The special treatment of flow in the matrix for a dual-permeability formulation where a vitric layer overlies a zeolitic layer is done by setting ISOT=-2 for the matrix to matrix connection between the vitric and the zeolitic elements. A small section of the input file (CONNE block) is shown in Figure 8. The vitric layer has a permeability of $1.60E-10$ m^2 while the zeolitic zone has a permeability of $6.00E-16$ m^2. In this case the modified weighting scheme used for flow calculations are based on downstream mobility.

For this problem, EOS9 is used to simulate the two-phase conditions. A constant influx rate is specified at the second element from the top. The output at steady-state are given below in Tables 34 and 35 showing that the saturations are very similar in the two simulations presented. The steady state mass flow rate for the various elements are given in Tables 36 and 37. The results between the modified and the previous qualified versions are similar, indicating a consistent performance of the codes.

```
ROCKS
ch1Mv   2 2300.     0.2650     0.1600E-110.1600E-110.1600E-11 1.200        1635.
                    1.2000
        7   0.2270  0.4000E-01 1.000     0.2000E-01           0.5000       5.086
        7   0.2270  0.4000E-010.9800E-040.1000E+11 1.000
ch1Mz   2 2300.     0.1930     0.6000E-170.6000E-170.6000E-17 1.200        1635.
                    1.2000
        7   0.3590  0.3600     1.000     0.2000E-01           0.5000       5.086
        7   0.3590  0.3600     0.1900E-060.1000E+11 1.000
ch1Fv   2 2300.     1.000      0.1740E-120.1740E-120.1740E-11 1.200        1635.
                    1.2000                                                 7.14E-5
        7   0.6330  0.1000E-01 1.000     0.2000E-01           0.5000       5.086
        7   0.6330  0.1000E-010.1180E-020.1000E+11 1.000
ch1Fz   2 2300.     1.000      0.2510E-130.2510E-130.2510E-12 1.200        1635.
                    1.2000                                                 1.10E-5
        7   0.6330  0.1000E-01 1.000     0.2000E-01           0.5000       5.086
        7   0.6330  0.1000E-010.1140E-020.1000E+11 1.000
REFCO      0.920E+05      25.00


ELEME
Fj425           ch1Fv0.2229E+060.1000E+01              172061.120234070.960 1128.7700
Mj425           ch1Mv0.1728E+060.0000E+00              172060.620234070.960 1128.7700
Fk425           ch1Fz0.3629E+060.1000E+01              172061.120234070.960 1073.1400
Mk425           ch1Mz0.3456E+060.0000E+00              172060.620234070.960 1073.1400
F1425           tswF40.2143E+060.1000E+01              172061.120234070.960 1017.5200
M1425           tswM40.1728E+060.0000E+00              172060.620234070.960 1017.5200
TP425           topbd0.4653E+040.0000E+00              172060.620234070.960 1231.8200
BT425           botbd0.4653E+540.0000E+00              172060.620234070.960  730.9700


CONNE
Fb425Fa425   0    0    0    30.3450E+010.3450E+010.4653E+040.1000E+01    1
Mb425Ma425   0    0    0    30.3450E+010.3450E+010.4653E+040.1000E+01    0
Fj425Fi425   0    0    0    30.1854E+020.3090E+010.4653E+040.1000E+01    1
Mj425Mi425   0    0    0    30.1854E+020.3090E+010.4653E+040.1000E+01    0
Fk425Fj425   0    0    0    30.3708E+020.1854E+020.4653E+040.1000E+01    1
Mk425Mj425   0    0    0   -20.3708E+020.1854E+020.4653E+040.1000E+01    0
F1425Fk425   0    0    0    30.1854E+020.3708E+020.4653E+040.1000E+01    1
M1425Mk425   0    0    0    30.1854E+020.3708E+020.4653E+040.1000E+01    0
Fs425Ms425   0    0    0    10.0000E+000.2488E+010.8175E+040.0000E+00    2
Ft425Mt425   0    0    0    10.0000E+000.2488E+010.3539E+050.0000E+00    2
Fu425Mu425   0    0    0    10.0000E+000.2488E+010.2697E+050.0000E+00    2
```

Figure 8. Selected input file for sample problem 9.

33

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.0528E-02
Ma425	9.20E+04	6.3472E-01
Fb425	9.20E+04	1.0540E-02
Mb425	9.20E+04	6.3661E-01
Fk425	9.20E+04	1.0035E-02
Mk425	9.20E+04	9.0926E-01
Fu425	9.20E+04	1.0066E-02
Mu425	9.20E+04	8.3499E-01
BT425	9.20E+04	9.9000E-01

Table 34. Steady state pressure and liquid saturation profiles obtained using the modified version of the EOS9 module for special treatment of the vitric/zeolitic interface.

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	1.09E+06	1.0528E-02
Ma425	9.20E+04	6.3431E-01
Fb425	9.20E+04	1.0540E-02
Mb425	9.20E+04	6.3619E-01
Fk425	9.20E+04	1.0042E-02
Mk425	9.20E+04	9.0923E-01
Fu425	9.20E+04	1.0065E-02
Mu425	9.20E+04	8.3499E-01
BT425	9.20E+04	9.9000E-01

Table 35. Steady state pressure and liquid saturation profiles obtained using the qualified version of the EOS9 module for special treatment of the vitric/zeolitic interface.

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.49071E-08
Mb425	Ma425	0.58686E-11
Mi425	Mh425	0.49130E-08
Mj425	Mi425	0.49130E-08
Mk425	Mj425	0.49130E-08
Ml425	Mk425	0.49130E-08
BT425	Mu425	0.49166E-08

Table 36. Steady-state liquid flow rate in kg/s obtained using the modified version of the EOS9 module.

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	0.49071E-08
Mb425	Ma425	0.58862E-11
Mi425	Mh425	0.49129E-08
Mj425	Mi425	0.49130E-08
Mk425	Mj425	0.49130E-08
Ml425	Mk425	0.49130E-08
BT425	Mu425	0.49130E-08

Table 37. Steady-state liquid flow rate in kg/s obtained using the qualified version of the EOS9 module.

4.2.5 Sample problem 10:
Post processing of TOUGH2 output

An additional subroutine for calculating the nodal velocities and fluxes has been developed. A sample problem was developed to check the output file, *tough2.tec*, for the values of velocities and fluxes at different nodes. A uniform two-dimensional mesh (10m x 10m x 1m) was generated using the MESHMAKER capabilities of the TOUGH2 code. The model problem consists of a two-dimensional flow domain with a constant isotropic permeability (k=0.8904 E-12 m^2) and a constant pressure difference of 1E+05 Pa applied across the two edges. The calculated velocity for this simple system is 0.8712E-06 m/s along the direction of the pressure gradient and zero across it and the results obtained from the simulations also gives the same value (Tables 38 and 39).

The input file for this problem is given in Figure 9.

```
TOUGH2    Run #1    1-D transport
2-d   flow for TEC  output
ROCKS
     1     3 1600.     1.e+00      .89040E-12 .8904e-12 .8904e-12 2.0000000   1.00e+03
0.000                              1.00000
3         .250        .250
     7          .250      .000     .0067E-4

PARAM            123456789012345678901234
 4 20300      030000000000001002030 0 5020    1.00e-05
0.00000E061.72800E16 1.000E+01 1.000e+04junkA        0.00000      3.0

1.500000000E+05         0.000000000000000     0.150000000000E+02
```

Figure 9. Selected input file for sample problem 10.

```
TIMES.
1
1.7280E06

MULTI
    2    3    2    8

RTSOL prec        rtol  info iplvl nitmx nort kacc  iredb
      1.0e-6        0.1    0    1   100   15    2     0
        1.e-4     2.e04        11.0       11.0         2.0        0.20        0.2    0




START

ELEME
A11 1               10.1000E+530.2000E+03            0.5000E+010.5000E+01-.5000E+00
A12 1               10.1000E+530.2000E+03            0.5000E+010.1500E+02-.5000E+00
A13 1               10.1000E+530.2000E+03            0.5000E+010.2500E+02-.5000E+00
.
.
.
A1910               10.1000E+530.2000E+03            0.9500E+020.8500E+02-.5000E+00
A1A10               10.1000E+530.2000E+03            0.9500E+020.9500E+02-.5000E+00


CONNE
A11 1A11 2               10.5000E+010.5000E+010.1000E+02
A11 1A12 1               20.5000E+010.5000E+010.1000E+020.0000E+00
.
.
.
A1710A1810              20.5000E+010.5000E+010.1000E+020.0000E+00
A1810A1910              20.5000E+010.5000E+010.1000E+020.0000E+00
A1910A1A10              20.5000E+010.5000E+010.1000E+020.0000E+00



INCON
A11 1           1.000000E+00
9.9000000000000E+05   0.000000000000E+00   0.1500000000E+02
A12 1           1.000000E+00
9.9000000000000E+05   0.000000000000E+00   0.1500000000E+02
.
.
A18 1           1.000000E+00
9.9000000000000E+05   0.000000000000E+00   0.1500000000E+02
A19 1           1.000000E+00
9.9000000000000E+05   0.000000000000E+00   0.1500000000E+02
A1A 1           1.000000E+00
9.9000000000000E+05   0.000000000000E+00   0.1500000000E+02
A1110           1.000000E+00
8.9000000000000E+05   0.000000000000E+00   0.1500000000E+02
A1210           1.000000E+00
8.9000000000000E+05   0.000000000000E+00   0.1500000000E+02   .
A1910           1.000000E+00
8.9000000000000E+05   0.000000000000E+00   0.1500000000E+02
A1A10           1.000000E+00
8.9000000000000E+05   0.000000000000E+00   0.1500000000E+02

ENDCY
```

Figure 9. Selected input file for sample problem 10 (contd.).

Eleme	Eleme	Liquid velocity	Liquid flow rate
		m/s	kg/s
A11 1	A11 2	-8.7121E-07	-8.7088E-03
A12 1	A12 2	-8.7121E-07	-8.7088E-03
A13 1	A13 2	-8.7121E-07	-8.7088E-03
A14 1	A14 2	-8.7121E-07	-8.7088E-03
A15 1	A15 2	-8.7121E-07	-8.7088E-03
A16 1	A16 2	-8.7121E-07	-8.7088E-03

Table 38. Flow velocity (m/s) and flow rate (kg/s) between two elements for some selected interfaces as obtained from the output of EOS3 module.

By selecting MOP(23)=2, TOUGH2 proceeds with the postprocessing of the state variables to calculate the velocity field in a format which can be used for plotting. The output is written to file, *tough2.tec*, and an abstracted version of the output file showing the liquid velocity and the mass flux in the x direction is given in Table 39. It may be pointed out that the output from TOUGH2 gives the total liquid flow rate across a given interface (Table 38) while the results from *tough2.tec* gives the fluxes (flow rate per unit area) as seen from Table 39.

X	Y	VLx	FMx
m	m	m/s	kg/s/m^2
5	5	8.7121E-07	0.00087088
5	15	8.7121E-07	0.00087088
5	25	8.7121E-07	0.00087088
5	35	8.7121E-07	0.00087088
5	45	8.7121E-07	0.00087088
5	55	8.7121E-07	0.00087088
5	65	8.7121E-07	0.00087088
5	75	8.7121E-07	0.00087088
5	85	8.7121E-07	0.00087088
5	95	8.7121E-07	0.00087088

Table 39. Liquid velocity in the x direction abstracted from the tough2.tec file for the two-dimensional flow problem.

4.2.6 Sample problem 11:
Transport module with dual permeability formulation (T2R3D)

The previously qualified version of T2R3D was developed for both the ECM and dual-permeability approaches for handling transport in fractured media (Wu et al., 1996). In the previous sections we have outlined several interface reduction schemes as the addition to the dual-permeability formulation for flow and transport. These modifications are identical to those discussed above for the EOS9 or EOS3 modules. In this section the T2R3D module is updated to incorporate the additional feature of transport in a dual-permeability media. The sample problem is designed for running the T2R3D code for the transport of a non-sorbing tracer. A one-dimensional grid with the dual permeability formulation is chosen. Transport of an ideal tracer under two-phase and non-isothermal conditions is simulated. Both inlet and outlet boundary conditions are specified to be at constant pressure, liquid saturation, radionuclide mass fraction and temperature by specifying a huge volume. Transport of the ideal tracer occurs through advection and molecular diffusion. The molecular diffusion coefficient is 1.0 E-10 m^2/s for the matrix and 1.0 E-13 m^2/s in the fractures.

The T2R3D module was setup for the one-dimensional problem to validate the revised version of the module. Figure 10 shows the input file for this problem. The mass fraction distribution of the tracer at each element at steady state is shown for the two versions of the code and they are identical (Tables 40 and 41). The flux rate calculations also give similar results (Table 42 and 43).

```
# input file for T2R3D module
ROCKS
tcwM1     2 2480.     0.6600E-010.5400E-170.5400E-170.5400E-17 1.730       935.8
                      1.7300     0.2500
          0.0      0.000.0000e+00        0.0  1.00e-10
     7      0.2310     0.1300     1.000     0.2000E-01            0.5000E-03 5.086
     7      0.2310     0.1300     0.1150E-050.1000E+11 1.000
.
.
tcwF1     2 2480.     1.000      0.6030E-110.6030E-110.2290E-09 1.730       935.8
                      1.7300     0.2500                                     2.33E-4
          0.0      0.000.0000e+00        0.0  1.00e-13
     7      0.6330     0.1000E-01 1.000     0.2000E-01            0.5000E-03 5.086
     7      0.6330     0.1000E-010.2370E-020.1000E+11 1.000

PARAM             123456789012345678901234
 4 20510     05101000000000002030    1400   0.00e-05
0.00000E003.15576E181.0000E+03              dummy     -9.80665    3.0
1.0000e-3
0.9282690278093E+05 0.1023955879578E+02 0.0000000000000E+00 0.2055102894970E+02
TIMES
1     1
3.15576E18
RTSOL prec        rtol info iplvl nitmx nort kacc  iredb
     1.0e-6       0.1   0    1   250   15    2     0
     1.e-5      1.e18     100.0      100.      1.30      0.20       0.2    1

MULTI
3     4     2     8
START

GENER  base-case present day infiltration (flint et al) /3
Fa425                            COM1 0.4913E-080.7561E+05 0.000E+00
```

Figure 10. Input file for sample problem 11 - T2R3D for dual-permeability.

```
ELEME
Fa425          tcwF10.8731E+550.1000E+01              172061.120234070.960 1228.3700
Ma425          tcwM10.3746E+550.0000E+00              172060.620234070.960 1228.3700
Fb425          tcwF20.1120E+060.1000E+01              172061.120234070.960 1221.4700
Mb425          tcwM20.3746E+050.0000E+00              172060.620234070.960 1221.4700
.
.
Fu425          ch3Fz0.2214E+050.1000E+01              172061.120234070.960  752.7400
Mu425          ch3Mz0.2013E+100.0000E+00              172060.620234070.960  752.7400
TP425          topbd0.4653E+540.0000E+00              172060.620234070.960 1231.8200
BT425          botbd0.4653E+540.0000E+00              172060.620234070.960  730.9700

CONNE
Fb425Fa425  0    0    0     30.3450E+010.3450E+010.4653E+040.1000E+01    1
Mb425Ma425  0    0    0     30.3450E+010.3450E+010.4653E+040.1000E+01    0
Fa425TP425  0    0    0     30.3450E+010.1000E-040.4653E+040.1000E+01    0
Ma425TP425  0    0    0     30.3450E+010.1000E-040.4653E+040.1000E+01    0
BT425Fu425  0    0    0     30.1000E-040.2177E+020.4653E+040.1000E+01    0
BT425Mu425  0    0    0     30.1000E-040.2177E+020.4653E+040.1000E+01    0
Fa425Ma425  0    0    0    +10.0000E+000.1634E+000.7644E+050.0000E+00    2
Fb425Mb425  0    0    0    +10.0000E+000.9107E-010.1371E+060.0000E+00    2
Fu425Mu425  0    0    0    +10.0000E+000.2488E+010.2697E+050.0000E+00    2

INCON—INITIAL CONDITIONS FOR    44 ELEMENTS AT TIME   0.247576E+14
Fa425                0.10000000E+01
0.8781396228567E+05 0.1098943479859E+02 1.0000000000000E-05 0.1504984671961E+02
0.1056520140997E-01 0.1056520140997E-01
Ma425                0.66000000E-01
0.8781396228567E+05 0.1023228719850E+02 1.0000000000000E-05 0.1504984671954E+02
0.7677128014996E+00 0.7677128014996E+00
Fb425                0.10000000E+01
0.8788526220303E+05 0.1098941318425E+02 0.0000000000000E+01 0.1514953987000E+02
0.1058681575041E-01 0.1058681575041E-01
Mb425                0.66000000E-01
0.8788524762308E+05 0.1022729569393E+02 0.0000000000000E+01 0.1514953986997E+02
0.7727043060728E+00 0.7727043060728E+00
TP425                0.90000000E+00
0.8777832356802E+05 0.1099893279823E+02 1.0000000000000E-05 0.1500000000000E+02
0.1067201765956E-02 0.1067201765956E-02
BT425                0.90000000E+00
0.9300000000000E+05 0.1000100000000E+02 0.0000000000000E+01 0.3200000000000E+02
0.9990000000000E+00 0.9990000000000E+00
ENDCY
```

Figure 10. Input file for sample problem 11 - T2R3D for dual-permeability (contd.).

Eleme	Tracer M.F.
Fa425	1.00E-05
Ma425	1.00E-05
Fb425	1.00E-05
Mb425	1.00E-05
Fu425	4.70E-48
Mu425	1.67E-07
TP425	1.00E-05
BT425	1.75E-53

Table 40. Mass fraction of the tracer at steady-state conditions for the modified T2R3D module.

Eleme	Tracer M.F.
Fa425	1.00E-05
Ma425	1.00E-05
Fb425	1.00E-05
Mb425	1.00E-05
Fu425	4.70E-48
Mu425	1.67E-07
TP425	1.00E-05
BT425	1.75E-53

Table 41. Mass fraction of the tracer at steady-state conditions for the qualified T2R3D module.

Eleme	Eleme	Liquid flow rate kg/s
Fb425	Fa425	4.9296E-09
Mb425	Ma425	1.4474E-07
Fr425	Fq425	7.0281E-11
Mr425	Mq425	1.5063E-07
Fs425	Fr425	1.2782E-10
Ms425	Mr425	1.5064E-07
Ft425	Fs425	3.1275E-10
Mt425	Ms425	1.5059E-07
Fu425	Ft425	6.0271E-10
Mu425	Mt425	1.5059E-07
BT425	Fu425	7.3533E-10
BT425	Mu425	1.5059E-07
Fa425	Ma425	-2.2955E-12
Fu425	Mu425	-6.5005E-13

Table 42. Liquid flow rate (kg/s) for the modified T2R3D module.

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	4.9296E-09
Mb425	Ma425	1.4474E-07
Fr425	Fq425	7.0281E-11
Mr425	Mq425	1.5063E-07
Fs425	Fr425	1.2782E-10
Ms425	Mr425	1.5064E-07
Ft425	Fs425	3.1275E-10
Mt425	Ms425	1.5059E-07
Fu425	Ft425	6.0271E-10
Mu425	Mt425	1.5059E-07
BT425	Fu425	7.3533E-10
BT425	Mu425	1.5059E-07
Fa425	Ma425	-2.2955E-12
Fu425	Mu425	-6.5005E-13

Table 43. Liquid flow rate (kg/s) for the qualified T2R3D module.

4.2.7 Sample problem 12:
Addition of a modified relative permeability model in the EOS1G module

A one-dimensional flow model is here used to validate the revised EOS1G module. As noted earlier a modified form of relative permeability function for two-phase condition is used which provides for greater interference between the liquid and the air phase. The model consists of 100 elements. The boundary condition is Dirichlet-type where the bottom boundary node is held at a constant pressure of 90 kPa. The input file is given in Figure 11. The propagation of the pressure pulse through the one-dimensional system is compared between the earlier version and the revised version of the codes. In the earlier qualified version, $k_{rg} = 1-k_{rl}$ whereas in the revised model an explicit form of the relative permeability to gas is obtained by using the modified form of the Brooks-Corey relation as discussed earlier.

The pressure profile after 1 day is shown below. Tables 44 through 47 compare the results between the revised version of EOS1G using the new relative permeability function and the qualified EOS1G code. The results show that the two versions give very similar results, with a maximum difference observed to be less than 0.2%. The position of the pressure front is also at the same position in both the results.

```
INPUT  sample for single-phase gas module (eos1g)
ROCKS
midle    3 2400.     0.01        1.000E-13 1.000E-13 1.000E-13 0.77119  1000.
0.000                            0.25
        7         .167   0.00            1.0                   1.0
        7         .167     .000      .1670E-4   .100E+13   .100E+01

topbd    3 2400.     0.01        1.000E-13 1.000E-13 1.000E-13 0.77119  1.0E+30
0.000                            0.25
        7         .167   0.00            1.0                   1.0
        7         .167     .000      .1670E-4   .100E+13   .100E+01
botbd    3 2400.     0.01        1.000E-13 1.000E-13 1.000E-13 0.77119  1.0E+30
0.000                            0.25
        7         .167   0.00            1.0
                    1.0      7        .167      .000      .1670E-4   .100E+13   .100E+01

PARAM               12345678901234567890234
 5 30555       05551000001 0040 203000 0       2.13e-05
               8.640E+04 7.200E+02                         9.80665      3.0
1.00E-05
0.5000000000000E+05 1.0250000000000E+01 2.5000000000000E+01

TIMES
1        1
3.15     E40
RTSOL prec        rtol info iplvl nitmx nort kacc   iredb
    1.0e-6         0.1    0    1   100   15    2     0
       1.e-0    1.e16      0.100           0.2       3.0       0.20        0.2      0

START
ELEME
AAA 1                2 1.000E+00
AAA 2    96     1    1 1.000E+00
AAA99                3 1.000E+50

CONNE
AAA 1AAA 2    97     1    1    3 0.500E+00 0.500E+00 1.000E+00 0.000E+00

INCON—INITIAL CONDITIONS FOR    99 ELEMENTS AT TIME   0.100000E+14
AAA99              0.10000000E-01
0.9000000000000E+05 0.1025000000000E+02 0.3000000000000E+02
ENDCY
```

Figure 11. Input file for sample problem 12- EOS1G module.

Eleme	Gas pressure
	Pa
AAA01	5.1320E+04
AAA02	5.1323E+04
AAA03	5.1330E+04
AAA04	5.1341E+04
AAA93	8.5146E+04
AAA94	8.5961E+04
AAA95	8.6773E+04
AAA96	8.7581E+04
AAA97	8.8384E+04
AAA98	8.9182E+04
AAA99	9.0000E+04

Table 44. Gas pressure at selected nodes (Pa) for the revised EOS1G module.

Eleme	Gas pressure
	Pa
AAA01	5.1201E+04
AAA02	5.1205E+04
AAA03	5.1212E+04
AAA04	5.1222E+04
AAA93	8.5314E+04
AAA94	8.6101E+04
AAA95	8.6885E+04
AAA96	8.7665E+04
AAA97	8.8440E+04
AAA98	8.9210E+04
AAA99	9.0000E+04

Table 45. Gas pressure at selected nodes (Pa) for the qualified EOS1G module.

Eleme	Eleme Gas	Velocity
		m/s
AAA01	AAA02	4.6475E-07
AAA02	AAA03	9.3055E-07
AAA03	AAA04	1.3985E-06
AAA04	AAA05	1.8696E-06
AAA95	AAA96	1.0565E-04
AAA96	AAA97	1.0502E-04
AAA97	AAA98	1.0429E-04
AAA98	AAA99	1.0648E-04

Table 46. Gas velocity at selected nodes (m/s) for the modified EOS1G module.

Eleme	Eleme	Gas Velocity
		m/s
AAA01	AAA02	4.6498E-07
AAA02	AAA03	9.3113E-07
AAA03	AAA04	1.3996E-06
AAA04	AAA05	1.8717E-06
AAA95	AAA96	1.0188E-04
AAA96	AAA97	1.0126E-04
AAA97	AAA98	1.0056E-04
AAA98	AAA99	1.0270E-04

Table 47. Gas velocity at selected nodes (m/s) for the qualified EOS1G module.

4.2.8 Sample problem 13:
Addition of a modified capillary pressure function near residual water saturation

The sample problem considers one-dimensional (1-D) vertical flow in the unsaturated zone where all the various elements consist of the same rock type. The boundary condition specified is Dirichlet-type conditions. The bottom boundary is treated as being at constant gas pressure, liquid saturation, and temperature by specifying a large volume. A liquid water source is introduced to the second element from the top to provide constant water infiltration. See Figure 12 for the input file where the modified capillary pressure function is designated by ICP=10 in the ROCKS card. The results of simulations are presented in Table 48-51. The simulation is allowed to reach steady-state. Tables 48 and 49 compare the pressure and liquid saturation in each element between the two versions of the code and show that the output is identical in both the cases. A similar conclusion is reached when the liquid fluxes are compared (Tables 50, 51).

```
# input file for   modified capillary pressure near residual water saturation
ROCKS
tcwM1    2 2480.     0.6600E-010.5400E-170.5400E-170.5400E-17 1.730       935.8
                    1.7300     0.2500
       7  0.2310    0.1300     1.000     0.2000E-01            0.5000E-03 5.086
      10  0.2310    0.1300     0.1150E-050.1000E-09 1.000
tcwF1    2 2480.     1.000     0.6030E-110.6030E-110.2290E-09 1.730       935.8
                    1.7300     0.2500                                     2.33E-4
       7  0.6330    0.1000E-01 1.000     0.2000E-01            0.5000E-03 5.086
      10  0.6330    0.1000E-010.1140E-020.1000E-09 1.000
topbd    2 2300.     0.2000     0.7472E-100.7472E-100.7472E-10 1.730      0.1000E+31

       1  0.2000    0.3000     0.7000     0.8000
       1                       1.000
botbd    2 2300.     0.2800     0.4700E-150.4700E-150.4700E-15 1.560      0.1000E+31
                    1.5600
       7  0.3900               1.000
      10  0.3900               0.5800E-060.1000E-09 1.000
REFCO    0.920E+05      25.00


PARAM             123456789012345678901234
 4 25100      510010000000000002030    1400   0.00e-05
0.00000E003.15576E181.0000E+01               dummy      -9.80665     3.0
 1.0000e-3
0.800       00E+00              .920e5              25.                  0.
TIMES
     1    1
3.15576E18

RTSOL prec      rtol info iplvl nitmx nort kacc  iredb
      1.0e-6      0.1   0    1   250   15   2    0
        1.e-5   1.e18     100.0      100.      1.30      0.20      0.2    1

START

GENER
Fa425                               COM1 0.4913E-060.7561E+05 0.000E+00


ELEME
Fa425          tcwF10.8731E+050.1000E+01        172061.120234070.960 1228.3700
Ma425          tcwM10.3746E+050.0000E+00        172060.620234070.960 1228.3700
Fb425          tcwF10.1120E+060.1000E+01        172061.120234070.960 1221.4700
Mb425          tcwM10.3746E+050.0000E+00        172060.620234070.960 1221.4700
Fr425          tcwF10.3543E+060.1000E+01        172061.120234070.960  852.1900
Mr425          tcwM10.7197E+050.0000E+00        172060.620234070.960  852.1900
```

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```
Fs425           tcwF10.6711E+040.1000E+01          172061.120234070.960  837.9000
Ms425           tcwM10.6101E+090.0000E+00          172060.620234070.960  837.9000
Ft425           tcwF10.2905E+050.1000E+01          172061.120234070.960  802.9200
Mt425           tcwM10.2641E+100.0000E+00          172060.620234070.960  802.9200
Fu425           tcwF10.2214E+050.1000E+01          172061.120234070.960  752.7400
Mu425           tcwM10.2013E+100.0000E+00          172060.620234070.960  752.7400
TP425           topbd0.4653E+040.0000E+00          172060.620234070.960 1231.8200
BT425           botbd0.4653E+540.0000E+00          172060.620234070.960  730.9700

CONNE
Fb425Fa425    0    0    0    30.3450E+010.3450E+010.4653E+040.1000E+01    1
Mb425Ma425    0    0    0    30.3450E+010.3450E+010.4653E+040.1000E+01    0
Fi425Mi425    0    0    0    10.0000E+000.1515E+000.6336E+050.0000E+00    2
Fj425Mj425    0    0    0   -10.0000E+000.1650E+000.3491E+060.0000E+00    2
Fk425Mk425    0    0    0   -10.0000E+000.2415E+000.4769E+060.0000E+00    2
Fl425Ml425    0    0    0    10.0000E+000.8865E-010.6497E+060.0000E+00    2
Fm425Mm425    0    0    0    10.0000E+000.9208E-010.3649E+060.0000E+00    2
Fn425Mn425    0    0    0    10.0000E+000.9208E-010.4170E+060.0000E+00    2
Fs425Ms425    0    0    0    10.0000E+000.2488E+010.8175E+040.0000E+00    2
Ft425Mt425    0    0    0    10.0000E+000.2488E+010.3539E+050.0000E+00    2
Fu425Mu425    0    0    0    10.0000E+000.2488E+010.2697E+050.0000E+00    2

INCON
Fa425              0.10000000E+01
   0.2155949292959E-01  0.9000000000000E+05  0.2155949292959E-01  0.2155949292959E-01
```

Figure 12. Input file for sample problem 13

Eleme	Pressure	Liq. Saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.1857E-02
Ma425	9.20E+04	6.3413E-01
Fb425	9.20E+04	1.1855E-02
Mb425	9.20E+04	6.3601E-01
Fc425	9.20E+04	1.1854E-02
Mc425	9.20E+04	6.3775E-01
Fi425	9.20E+04	1.1852E-02
Mi425	9.20E+04	6.5665E-01
Fj425	9.20E+04	1.1852E-02
Mj425	9.20E+04	6.6366E-01
Fk425	9.20E+04	1.1852E-02
Mk425	9.20E+04	6.8376E-01
Ft425	9.20E+04	1.1827E-02
Mt425	9.20E+04	8.6899E-01
Fu425	9.20E+04	1.1582E-02
Mu425	9.20E+04	9.3990E-01
BT425	9.20E+04	9.9000E-01

Table 48. Pressure and liquid saturation profiles obtained using the modified capillary function near residual water saturation with the EOS9 module at steady-state conditions.

Eleme	Pressure	Liq. saturation
	Pa	
TP425	9.20E+04	1.0000E-02
Fa425	9.20E+04	1.1857E-02
Ma425	9.20E+04	6.3415E-01
Fb425	9.20E+04	1.1855E-02
Mb425	9.20E+04	6.3602E-01
Fc425	9.20E+04	1.1854E-02
Mc425	9.20E+04	6.3776E-01
Fi425	9.20E+04	1.1852E-02
Mi425	9.20E+04	6.5666E-01
Fj425	9.20E+04	1.1852E-02
Mj425	9.20E+04	6.6367E-01
Fk425	9.20E+04	1.1852E-02
Mk425	9.20E+04	6.8377E-01
Ft425	9.20E+04	1.1828E-02
Mt425	9.20E+04	8.6899E-01
Fu425	9.20E+04	1.1560E-02
Mu425	9.20E+04	9.3990E-01
BT425	9.20E+04	9.9000E-01

Table 49. Pressure and liquid saturation profiles obtained using the qualified version of the EOS9 module at steady-state conditions.

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	4.9071E-07
Mb425	Ma425	5.8548E-10
Fc425	Fb425	4.8886E-07
Mc425	Mb425	2.4372E-09
Fd425	Fc425	4.8821E-07
Md425	Mc425	3.0928E-09
Fe425	Fd425	4.8777E-07
Me425	Md425	3.5335E-09
Fi425	Fh425	4.8682E-07
Mi425	Mh425	4.4822E-09
Fj425	Fi425	4.8638E-07
Mj425	Mi425	4.9229E-09
Fk425	Fj425	4.8635E-07
Mk425	Mj425	4.948E-09
Fr425	Fq425	4.6741E-07
Mr425	Mq425	2.3885E-08
Fs425	Fr425	4.6512E-07
Ms425	Mr425	2.6184E-08
Ft425	Fs425	4.6511E-07
Mt425	Ms425	2.6185E-08
Fu425	Ft425	4.6511E-07
Mu425	Mt425	2.6188E-08
BT425	Fu425	4.6511E-07
BT425	Mu425	2.6189E-08

Table 50. Liquid flow rate obtained using the modified capillary function near residual water saturation with the EOS9 module at steady-state conditions.

Eleme	Eleme	Liquid flow rate
		kg/s
Fb425	Fa425	4.9071E-07
Mb425	Ma425	5.8758E-10
Fc425	Fb425	4.8885E-07
Mc425	Mb425	2.4458E-09
Fd425	Fc425	4.8820E-07
Md425	Mc425	3.1038E-09
Fe425	Fd425	4.8775E-07
Me425	Md425	3.5460E-09
Fi425	Fh425	4.8680E-07
Mi425	Mh425	4.4984E-09
Fj425	Fi425	4.8636E-07
Mj425	Mi425	4.9409E-09
Fk425	Fj425	4.8633E-07
Mk425	Mj425	4.9661E-09
Fr425	Fq425	4.6725E-07
Mr425	Mq425	2.4047E-08
Fs425	Fr425	4.6492E-07
Ms425	Mr425	2.6376E-08
Ft425	Fs425	4.6492E-07
Mt425	Ms425	2.6377E-08
Fu425	Ft425	4.6492E-07
Mu425	Mt425	2.6380E-08
BT425	Fu425	4.6492E-07
BT425	Mu425	2.6380E-08

Table 51. Liquid flow rate obtained using the qualified version of the EOS9 module at steady-state conditions.

Requirement	Test Case	Criteria Met?	Reference
ECM/EOS3 Module			
sample problem to illustrate code,verify accuracy	1	Yes	this paper
heterogeneous property input	2	yes	this paper
EOS9 Module dual-k with various interface area reduction factor			this paper
reduction by upstream liquid saturation (ISOT=-1)	3	yes	this paper
reduction factor is upstream relative permeability times a constant factor (ISOT=-3)	4	yes	this paper
reduction factor is upstream relative permeability (ISOT=-4)	5	yes	this paper
reduction factor is normalized mass flux (ISOT=-7)	6	yes	this paper
reduction factor is normalized mass flux time supstream liquid saturation (ISOT=-8)	7	yes	this paper
reduction factor is constant factor (ISOT=-9)	8	yes	this paper
Modified weighting scheme for vitrc/zeolitic interface (ISOT=-2)	9	yes	this paper
Post-procesing of output	10	yes	this paper
T2R3D dual-k	11		this paper
EOS1G modified realtive permeability	12	yes	this paper
EOS9 modified capillary pressure function near residual water saturation	13	yes	this paper

Table 52. Requirements Validation Cross-Check

5. Software User Documentation

Input and Output

5.1 Single-Phase Gas Flow Module (EOS1G)

Input and output files, file formats, options, default parameters, data files, commands, and execution for this module are the same as described for the TOUGH2 EOS3 module in section 5.3 of Pruess et al. (1996). The modified form of the relative permeability to the gas phase is input through record "ROCKS" in the TOUGH2 code, and the related modifications in input data are read in card ROCKS.1.2

Card ROCKS.1.2   (I5,5X,7E10.4) IRP, RP(i), i=1, 7
IRP=   7   for the modified form of relative permeability to gas
RP(1)=   m   van Genuchten parameter (Eq. 11)
RP(2)= S_{lr} residual liquid saturation (Eq. 10)
RP(3)= S_{max} maximum liquid saturation (Eq. 10)

5.2 Interface area reduction scheme in module EOS9 or EOS3 or T2R3D

For the unsaturated/saturated flow in dual-permeability media, the input data and formats are the same as those for the TOUGH2 EOS3, EOS9 and T2R3D module (Pruess, 1987, 1991; Wu et al., 1996), except the following changes in CONNE and ELEME blocks. These changes in ISOT value are made for the corresponding fracture-matrix connections only.

Card CONNE.1   (A3, I2, A3, I2, 4I5, 4E10.4) EL1, NE1, EL2, NE2, NSEQ, NAD1, NAD2, ISOT, D1, D2, AREAX, BETAX

ISOT is set to -1, -3, -4, -7, -8, or -9 for the corresponding scenarios as discussed before.

We also need a change in the following ELEME card:
Card ELEME.1   (A5, 10X, A3, A2, 2E10.4, 10x, 3F10.3) ELEM, MA1, MA2, VOLX, AHT, X, Y, Z

Here AHT is used as an identifier for fracture elements. AHT > 0 is for fracture elements in the dual-permeability simulations. AHT=0 or default is used for non dual-permeability runs, and is for matrix elements for a dual-permeability grid. X, Y, Z are coordinates of the center of the element.

5.3 Modified weighting scheme at vitric/zeolitic interface

For the dual-permeability formulation, a special scheme only for the matrix-matrix connection is implemented when a vitric layer overlies a zeolitic layer. The following change is implemented in CONNE block for the ISOT value.

Card CONNE.1   (A3,I2,A3,I2, 4I5, 4E10.4) EL1, NE1, EL2, NE2, NSEQ, NAD1, NAD2, ISOT, D1, D2, AREAX, BETAX

ISOT is set to −2 to invoke this option.

5.4 Output files for visualization

Formatted outputs of fluid velocities and mass fluxes which can be used directly by commercial visualization softwares are now available in TOUGH2. This feature is enabled by using the PARAM.1 card and the following changes.

(a)   Card PARAM.1   (2I2, 3I4, 24I1, 2E10.4) NOITE, KDATA, MCYC, MSEC, MCYPR, (MOP(I), I=1, 24), DIFF0, TEXP

MOP(23)=   0,   no postprocessing option.

MOP(23)=   1,   postprocessing of primary variables like pressures, saturations, temperature, capillary pressure written to a file, **tough2.tec**.

MOP(23)=   2,   postprocessing of primary variables, in addition, pore velocities and mass fluxes at the nodes written to a file, **tough2.tec**.

MOP(24)=   0,   single continuum or ECM flow field, in which case all the results written to a file **tough2.tec** only.

MOP(24)=   1,   for dual-permeability flow fields, in which case besides the **tough2.tec** which represents the matrix variables, an additional output file **tough_f.tec** for the fracture continuum is also written.

(b)   Card ELEME.1   (A5, 10X, A3, A2, 2E10.4, 10x, 3F10.3) ELEM, MA1, MA2, VOLX, AHT, X, Y, Z

Here AHT is used as an identifier for fracture elements.   AHT > 0 is for fracture elements in the dual-permeability simulations, and AHT=0 or default is used for matrix or single-continuum elements.

(c)   Card CONNE.1   (A3, I2, A3, I2, 4I5, 4E10.4, I5) EL1, NE1, EL2, NE2, NSEQ, NAD1, NAD2, ISOT, D1, D2, AREAX, BETAX, IFM_CON

Here parameter IFM_CON identifies if the connection is fracture-fracture, fracture-matrix, or matrix to matrix. IFM_CON=0 or default is used for single-continuum or ECM block connection, and is for matrix-matrix connection in a dual-permeability grid. IFM_CON=1 is for fracture-fracture connection and IFM_CON=2 for fracture-matrix connection of a dual-permeability grid, respectively.

5.5 Data Input for spatially varying rock properties

The modifications required in EOS3, EOS9 and T2R3D modules to read in the spatially varying parameters corresponding to each element of the flow field is as follows:

Keyword **SVPAR** in the input file which can be placed anywhere after the keyword START but before ENDCY. The input file **svparam.dat** is needed, where the values of porosity, rock density and specific heat are given for each element with format (10X,3E10.4).

5.6 Brooks-Corey Relative Permeability function

The modified form of the relative permeability to the liquid and gas phase is input through record "ROCKS" in the TOUGH2 code, and the related modifications in input data are read in card ROCKS.1.2

Card ROCKS.1.2   (I5,5X,7E10.4) IRP, RP(i), i=1, 7
IRP =   12   for the modified form of relative permeability to gas
RP(1) = S_{lr} residual liquid saturation van Genuchten parameter (Eq. 10)
RP(2) = S_{gr} residual gas saturation (Eq. 10)
RP(3) =   m   van Genuchten soil characteristic parameter (Eq. 11)
RP(4) >   0.0   for $k_{rg} = 1 - k_{rl}$ (Eq. 8)
        <= 0.0   for Brooks-Corey function (Eq. 9)

5.7 Modified Capillary pressure function near residual water saturation

The modified form of the capillary pressure function is input through record "ROCKS" in the TOUGH2 code, and the related modifications in input data are read in card ROCKS.1.3

Card ROCKS.1.3   (I5,5X,7E10.4) ICP, CP(i), i=1, 7
ICP =   10   for the modified form of capillary pressure function
CP(1) =   m   van Genuchten soil characteristic parameter
CP(2) = S_{lr} residual liquid saturation
CP(3) = α related to P_o, air entry pressure (Pa), [1/CP(3)]
CP(4) =   e   small number (default=1.0e-5)
CP(5) = S_{ls} maximum liquid saturation

6. Summary and Conclusions

The modifications and additions to the selected TOUGH2 modules are verified, including the ECM/EOS3, EOS9, EOS1G and T2R3D modules. Verification of this phase of the Software Life Cycle, relating to user documentation and code demonstration cases, was completed by providing with this package the sample problems described in this report. These problems also demonstrate how the user sets up certain types of problems and explore various aspects and applications of the code. Certain enhancements to the code to allow for postprocessing of the output for plotting of fluxes and velocities, and addition of new relative permeability functions have also been documented.

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Appendix A. List of input and output files

All the 12 sample problems discussed in the text have been put on a diskette for ease of reference. The following table provides a list of the files that are available on the diskette, and it includes both the input and the output file for each of the sample problems.

Problem description	Revised version Input file	Revised version Output file	Previously qualified version Input file	Previously qualified version Output file
EOS3/ECM	prob1a.dat	prob1a.out	prob1b.dat	prob1b.out
EOS3/ECM spatially varying data	prob2a.dat	prob2a.out	prob2b.dat	prob2b.out
EOS9- dual k fracture-matrix interaction ISOT=-1	prob3a.dat	prob3a.out	prob3b.dat	prob3b.out
EOS9- dual k fracture-matrix interaction ISOT=-3	prob4a.dat	prob4a.out	prob4b.dat	prob4b.out
EOS9- dual k fracture-matrix interaction ISOT=-4	prob5a.dat	prob5a.out	prob5b.dat	prob5b.out
EOS9- dual k fracture-matrix interaction ISOT=-7	prob6a.dat	prob6a.out	prob6b.dat	prob6b.out
EOS9- dual k fracture-matrix interaction ISOT=-8	prob7a.dat	prob7a.out	prob7b.dat	prob7b.out
EOS9- dual k fracture-matrix interaction ISOT=-9	prob8a.dat	prob8a.out	prob8b.dat	prob8b.out
EOS9- dual k vitric/zeolitic interface modified weighting ISOT=-2	prob9a.dat	prob9a.out	prob9b.dat	prob9b.out
Post-processing for velocity and fluxes	prob10.dat	prob10.out		
T2R3D transport in dual k	prob11a.dat	prob11a.out	prob11b.dat	prob11b.out
EOS1G	prob12a.dat	prob12a.out	prob12b.dat	prob12b.out
EOS9 modified capillary pressure function near residual water saturation	prob13a.dat	prob13a.out	prob13b.dat	prob13b.out

Appendix B. TOUGH2 code source files

The revised and updated versions of the software constituting version 1.3 of TOUGH2 have been put together on a diskette. All the souce code for TOUGH2 are available on 3.5" high-density diskette, written in PC-DOS ASCII format. The distribution includes the following 19 files :

The following is a list of the files that are available:

1. t2cgn2.f	contains the main program of TOUGH2, with PARAMETER statements and initialization of disk files
2. meshmn.f	module with internal mesh generation facilities
3. eos3ecm.f	equation of state for water/air with ECM option
4. eos9ecm.f	equation of sate for water/air with air treated as a passive phase and ECM option
5. eos32l.f	equation of state for water, air and radionuclide
6. eos1g.f	equation of state for water/air with water treated as a passive phase
7. t2fecm.f	modified to include ECM option from 2f.f of TOUGH2 Version 1.11; it reads input data, initializes arrays and parameters, sets up Newton-Raphson iteration, and performs time stepping; it also contains the water property routines (steam table equations) and the relative permeability and capillary pressure functions which are used in the equation-of-state modules
8. t2f2l2.f	similar to t2fecm.f used in the T2R3D module
9. t2fecm1g.f	similar to t2fecm.f used in the eos1g module
10. inter.f	an iterative sparse matrix solver for block matrices (Copyrighted)
11. relpecm.f	evaluating relative permeability with ECM option
12. relp1g.f	evaluating relative permeability for EOS1G
13. pcapecm.f	evaluating capillary pressure with ECM option
14. sndibm.f	computing time subroutine
15. corder.f	subroutine to sort indexes of all connections for each element, used in T2R3D
16. diffd.f	subroutine to calculate hydraulic dispersion and molecular diffusion tensor, used in T2R3D
17. gradx.f	subroutine to calculate concentration gradients, used in T2R3D
18. tough2.prm	Parameter 'INCLUDE' file to set up dimensions of arrays used in the TOUGH2 code
19. matb.com	Parameter file for the solver

Source codes for the different TOUGH2 modules

The TOUGH2 EOS3/ECM module:
t2cgn2.f
t2fecm.f
meshmn.f
eos3ecm.f
relpecmn.f
inter.f
pcapecm.f
pcapgen.f
sndibm.f
tough2.prm
matb.com

The TOUGH2 EOS1G module:
t2cgn2.f
t2fecm1g.f
meshmn.f
eos1g.f
relp1g.f
inter.f
pcapecm.f
pcapgen.f
sndibm.f
tough2.prm
matb.com

The TOUGH2 EOS9 module:
t2cgn2.f
t2f_9.f
meshmn.f
eos9_up.f
relpecmn.f
inter.f
pcapecm.f
sndibm.f
tough2.prm
matb.com

The TOUGH2 T2R3D module
t2cgn2.f
t2f2l2.f
meshmn.f
eos32l.f
relpecmn.f
inter.f
pcapecm.f
pcapgen.f
sndibm.f
gradx.f
diffd.f
corder.f
tough2.prm
matb.com