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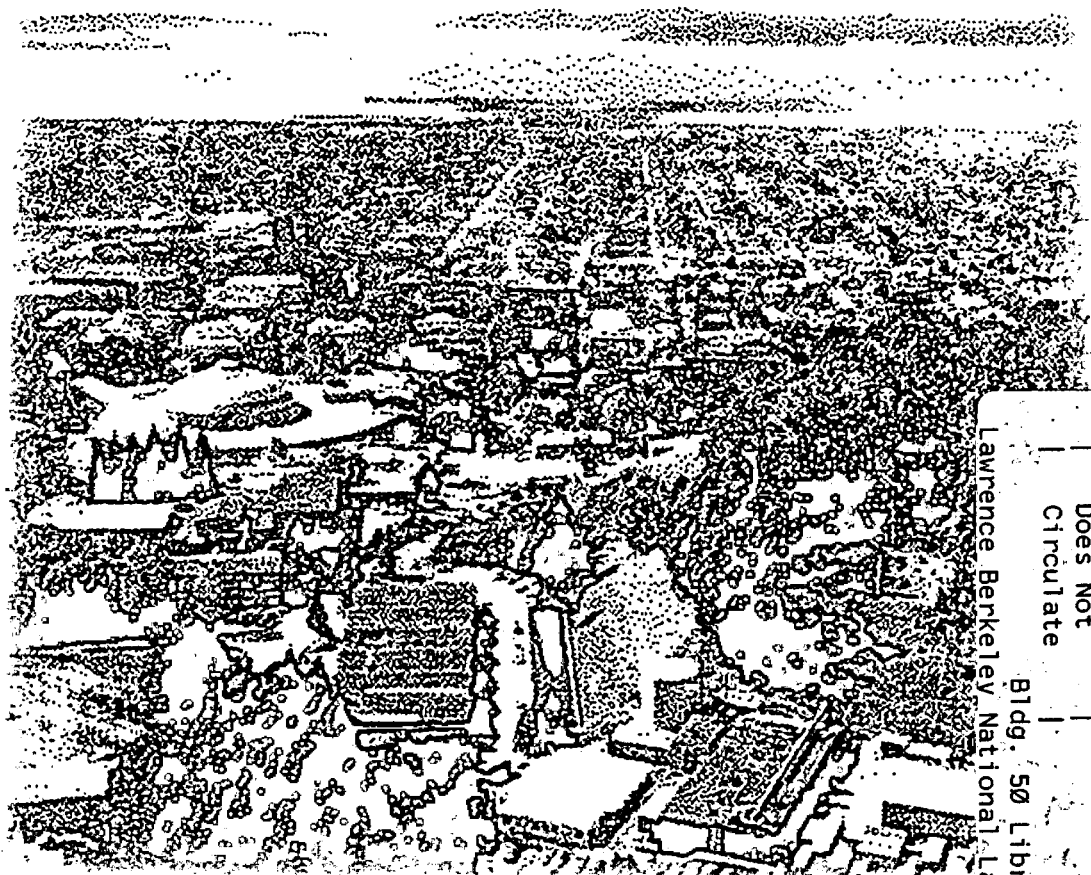


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## Software Qualification of Selected TOUGH2 Modules

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A. Simmons, and K. Pruess  
**Earth Sciences Division**

October 1996



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**SOFTWARE  
QUALIFICATION  
OF SELECTED  
TOUGH2  
MODULES**

TOUGH2

TOUGH2

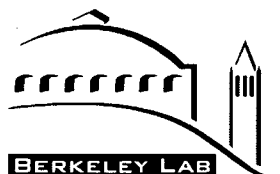
TOUGH2

TOUGH2

TOUGH2

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OCTOBER 1996



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THIS WORK WAS PREPARED UNDER THE OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT, U.S. DEPARTMENT OF ENERGY CONTRACT NO. DE-AC03-76SF00098, AND DE-A108-78ET44802 ADMINISTERED BY THE NEVADA OPERATIONS OFFICE IN COOPERATION WITH THE U.S. GEOLOGICAL SURVEY, DENVER

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# 1. INTRODUCTION

## Software Qualification

The purpose of this package of reports is to provide all software baseline documents necessary for the software qualification of the single-phase Gas (EOS1G), Effective Continuum Method (ECM), Saturated/Unsaturated Flow (EOS9), and Radionuclide Transport (T2R3D) modules of TOUGH2, 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 predecessor document, the *TOUGH2 Software Qualification* (Pruess et al., 1996).

In accordance with Yucca Mountain Project (YMP) / Lawrence Berkeley National Laboratory (LBNL) Quality Implementing Procedure YMP-LBNL-QIP-SI.0, *Software Qualification*, all components of the specified baseline documentation are provided. The software is not acquired, therefore no parts of the documentation are exempt from software verification and validation. This report contains the following sections: 1) Requirements Specification, 2) Design Description, 3) Software Validation Test Plan and Report, 4) Software User Documentation, and 5) Appendices. These sections comprise sequential parts of the Software Life Cycle, and are not intended to stand alone but should be used in conjunction with the *TOUGH User's Guide* (Pruess, 1987), *TOUGH2 - A General Purpose Numerical Simulator for Multiphase Fluid and Heat Flow* (Pruess, 1991), and the above-referenced TOUGH2 software qualification document. The qualification package is complete with the attached Software Identification Form and executable source code for the single-phase Gas, Effective Continuum Method, Saturated/Unsaturated Flow, and Radionuclide Transport modules of TOUGH2.

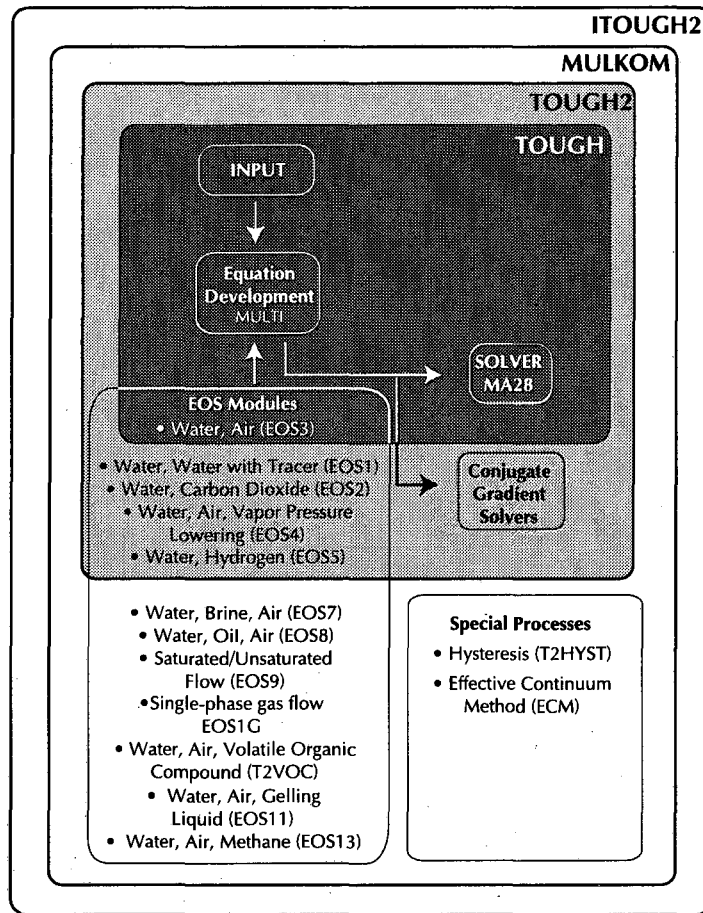
The version of TOUGH2 used with the software being qualified herein is the November 1994 Standard Version 1.11, as qualified in Pruess et al. (1996) and housed at the Department of Energy's Energy Science and Technology Software Center (ESTSC) in Oak Ridge, Tennessee. The qualification status of TOUGH2 related software is shown in Figure 1.

Previously Qualified (Pruess et al., 1996)	Qualified in Finsterle et al., 1996	Qualified Herein	To Be Qualified
TOUGH2	ITOUGH2	Single-Phase Gas (EOS1G)	Hysteresis (T2HYST)
Water, Water with Tracer (EOS1)		Effective Continuum Method (ECM)	Semianalytical Dual- Porosity Model
Water, Carbon Dioxide (EOS2)		Saturated/Unsaturated Flow (EOS9)	
Water, Air (EOS3)		Radionuclide Transport (T2R3D)	
Water, Air, Vapor Pressure Lowering (EOS4)			
Water, Hydrogen (EOS5)			

Figure 1. Qualification status of TOUGH2 related software.

## Background: 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 (“MULTi-KOMponent”) 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 relationship of TOUGH, TOUGH2 and ITOUGH2 to the MULKOM architecture is shown in Figure 2.



*Figure 2. Relationship of TOUGH, TOUGH2 (and modules) and ITOUGH2 to the MULKOM architecture.*

The remainder of this document is structured to address the TOUGH2 modules in a parallel fashion. Each of the four sections contains separate parts for each of the components under examination.

### Description: The Single-Phase Gas Flow Module of TOUGH2 (EOS1G)

The single-phase gas flow module (Equation-of-State 1G, or EOS1G) of the TOUGH2 code is used for efficient simulation of gas flow under gas and water (two-phase) flow conditions, where water is treated as a passive phase and the system is subject to non-uniform but stable moisture and geothermal conditions. To simulate these processes, the single-phase module uses

the same description of the physical processes of multi-phase flow in saturated and unsaturated heterogeneous media.

Description: The Effective Continuum Method Formulation Module of TOUGH2 (ECM)

When considering flow in fractured porous media, the key issue is how to evaluate inter-fluid exchange between matrix blocks and surrounding fractures. The available evaluation methods include: (1) explicit discrete fracture and matrix treatment; (2) effective continuum method; (3) double porosity method; (4) dual-permeability method; and (5) multiple interacting continua (MINC) method (Pruess and Narasimhan, 1985). The TOUGH2 code provides each of these options for treatment of fracture and matrix flow, but the ECM approach has found wide application because of its simplicity in terms of data requirements and computational intensity. The MINC treatment was addressed in the qualification of TOUGH2, v. 1.11 (Pruess et al. 1996), while the ECM treatment is qualified herein.

Description: The Saturated/Unsaturated Flow Module of TOUGH2 (EOS9)

The saturated/unsaturated flow module (equation-of-state 9, or EOS9) of the TOUGH2 code is used for efficient simulation of liquid flow under water and gas (two-phase) and water only (single-phase) flow conditions, where gas may be treated as a passive phase, and the system is subject to variable saturation but isothermal (single temperature) conditions. To simulate these processes, the EOS9 module uses a Richard's equation approximation (1931) for the physical processes of multi-phase flow in saturated and unsaturated heterogeneous media.

Description: The Radionuclide Transport Module of TOUGH2 (T2R3D)

T2R3D is a TOUGH2 module for modeling the transport of radio-nuclides or liquid tracers in non-isothermal, three-dimensional multiphase subsurface systems. The code was designed to simulate processes of radionuclide transport in the liquid phase by advection, molecular diffusion and hydrodynamic dispersion mechanisms. T2R3D can handle general transport problems using an irregular, 3-D integral finite difference grid.

## 2. REQUIREMENTS SPECIFICATION

This section describes specific requirements for each item being qualified through this report, and should be considered in addition to those previously covered for TOUGH2 in Pruess et al. (1996).

### Single-Phase Gas Flow Module (EOS1G)

The single-phase gas flow module of the TOUGH2 code must provide an accurate description of gas flow dynamics and constitutive physical laws and properties affecting the gas phase. It also must be capable of handling different geometries in one, two, and three dimensions, and rapidly-changing surface atmospheric conditions. The single-phase gas flow module differs from the previously-qualified module of TOUGH2 Version 1.11 used for gas flow, EOS3, in one way: it solves the conservation equation of the air component only, instead of including water mass and energy balance equations. Otherwise, all capabilities of the TOUGH2 code are preserved in this module. Verification and validation tests have been performed that collectively address all of the requirements listed in Section 2.1 for this module.

### Effective Continuum Method Formulation Module (ECM)

The effective continuum approach can accommodate two-phase flow in a fracture/matrix system, and this method is based on an assumption that local thermodynamic equilibrium exists between the fracture and matrix system (Pruess et al., 1990). When applicable, it provides a substantial simplification of description of fluid and heat flow in fractured porous media. The favorable conditions for this method are when rock matrix blocks are relatively small and permeable and the fracture network is relatively uniformly distributed. However, the effective continuum approximation may break down under certain unfavorable conditions, such as for a very tight, large and low-permeability rock matrix with rapid transient flow, because it may take a long time to reach equilibrium conditions under such an environment. The continuum method will be particularly suitable for a situation when a long-term, averaged, or steady-state solution is sought.

### Saturated/Unsaturated Flow Module (EOS9)

Like the single-phase gas flow module described above, the saturated/unsaturated flow module of TOUGH2 must provide an accurate description of flow dynamics and constitutive physical laws and properties affecting a single phase, in this case the liquid phase. It also must be capable of handling different geometries in one, two, and three dimensions. The saturated/unsaturated flow module differs from the previously-qualified module of TOUGH2 Version 1.11 (Pruess et al., 1996) used for liquid flow, EOS3, in one way: it solves the conservation equation for the liquid mass component only, and does not include the gas mass and energy balance equations. Otherwise, all capabilities of the TOUGH2 code are preserved in this module. Verification and validation tests have been performed that collectively address all of the requirements listed in Section 2.1 for this module.

### Radionuclide Transport Module (T2R3D)

The objective of this module is to provide a numerical tool to handle radionuclide or tracer transport in a non-isothermal multi-phase flow environment, including fracture-matrix interaction. The numerical method for this transport module is based on the integral finite difference scheme, as in the TOUGH2 code. The major assumptions of the radionuclide transport module are: (a) a radionuclide or a tracer exists and is transported only within the liquid phase, (b) transport mechanisms include molecular diffusion and hydrodynamic dispersion in the liquid phase in

addition to advection, and (c) first order decay and linear adsorption on rock grains are taken into account. The radionuclide or tracer is introduced as an additional mass component into the standard TOUGH2 formulation.

## 2.1 Requirements

### Single-Phase Gas (EOS1G) and Saturated/Unsaturated Flow (EOS9) Module Requirements

- A. Flow processes driven by pressure, viscous, capillary, and gravity forces
  - single-phase gas flow in two-phase existing conditions (EOS1G)
  - single-phase water flow in two-phase or single-liquid phase conditions (EOS9)
- B. Physics
  - accurate description of thermophysical properties of water, vapor, and air
  - dissolution of air in water
- C. Phase change and interaction
  - interference between liquid and gas phases
- D. Constant, but non-uniform temperature distribution (EOS1G)
- E. Dimensionality
  - 1-D, 2-D, and 3-D flows
- F. Geometry
  - Cartesian, cylindrical, irregular
- G. Grid generation
- H. Heterogeneities
  - heterogeneous formations
  - flow in porous and fractured media
- I. Flexible specification of initial and boundary conditions, sources and sinks
- J. Other
  - automatic time-stepping
  - restart capability
  - sample problems to illustrate code use and verify accuracy
  - internal version control

### Effective Continuum Method Formulation (ECM) Module Requirements

- A. Constitutive relations: accurate description of relative permeability and capillary pressure functions under local thermodynamic equilibrium assumption.

### Radionuclide Transport (T2R3D) Module Requirements

- A. Flow processes driven by pressure, viscous, capillary, and gravity forces
  - two-phase flow of liquid and gas (air and vapor)
- B. Physics
  - accurate description of thermophysical properties of water, vapor, and air
  - binary diffusion of air and water components in gas phase
  - binary diffusion and hydrodynamic dispersion of radionuclides in liquid phase
- C. Phase change and interaction
  - appearance and disappearance of phases
  - interference between liquid and gas phases
  - enhancement of gas phase permeability from Knudsen (slip flow) effects
  - vapor-liquid phase change
- D. Heat transport
  - heat conduction
  - heat convection

- sensible and latent heat changes
- conductive heat exchange with impermeable strata
- coupled fluid and heat flow
- E. Dimensionality
  - 1-D, 2-D, and 3-D flows
- F. Geometry
  - Cartesian, cylindrical, irregular
- G. Grid generation
- H. Heterogeneities
  - heterogeneous formations
  - flow in porous and fractured media
- I. Flexible specification of initial and boundary conditions, sources and sinks
- J. Other
  - automatic time-stepping
  - restart capability
  - sample problems to illustrate code use and verify accuracy
  - internal version control
  - modularized structure for modifying or adding capabilities

## 2.2 Prior Examples of Requirements 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, coupling between fluid and heat flows, and complexity of boundary conditions. These results, as well as additional verification and validation problems for the MULKOM/TOUGH codes, substantiate the accuracy of the process description employed in the code, and the mathematical and numerical approaches used. See Sections 2.2 and 2.2.1 of Pruess et al. (1996) for a full discussion of related examples, including those specifically applicable to nuclear waste disposal.

### Single-Phase Gas Flow Module (EOS1G)

There are no formally published example problems for verification of this new module. Therefore a verification example is provided in Section 4 of this report, which compares the simulation results from the single-phase gas flow module with those from the validated TOUGH2-EOS3 program.

### Effective Continuum Method Formulation Module (ECM)

The ECM formulation, as implemented in the TOUGH2 code, is a theory for treating fracture and matrix flow. The theory is based on the assumption that a local thermodynamic equilibrium exists between fracture and matrix systems, and in general it cannot be validated for various applications. As long as the flow condition for a given problem satisfies the assumption, the ECM scheme will give an accurate description of the fracture/matrix interactions of the system. In order to check the accuracy of the ECM scheme, we will provide an example in Section 4 of this report which compares the simulation results of the ECM and the dual-permeability modeling approaches.

### Saturated/Unsaturated Flow Module (EOS9)

The TOUGH2 EOS9 module has been verified and used at LBNL since the early 1990's (Pruess et al., 1996), but it has not been formally documented. In Section 4 of this report, we will present a verification example using the validated TOUGH2 EOS3 module and a semi-analytical solution to examine the simulation results of the TOUGH2 EOS9 module.

### Radionuclide Transport Module (T2R3D)

The T2R3D program is a new addition to the TOUGH2 family of codes, and no verification examples have been published yet. In Section 4 of this report, we will present two verification examples, for one- and two-dimensional transport problems.

### 3. DESIGN DESCRIPTION

This section describes the formal structure and architecture of the Single-Phase Gas, Effective Continuum Method, Saturated/Unsaturated Flow, and Radionuclide Transport modules of TOUGH2. It details the functional requirements of the software and how they are implemented. It explains how the modules handle the physics of the processes modeled, provides a description of numerical models and methods, describes the software structure, logic, and data structure and flow, and includes performance requirements and design constraints.

Topics related to sections 3.5-3.14 (handling of arrays, specification of setup, etc.) are not applicable to the ECM formulation module because the ECM module is a sub-routine carried out within TOUGH2. Considerations of code design and structure, therefore, refer to TOUGH2. For this the reader should consult Pruess et al. (1996).

Refer to the corresponding section and subsections of Pruess et al. (1996) for information and background materials related to the overall design, structure, and architecture of the TOUGH2 code and previously qualified modules.

#### 3.1 Design Background of TOUGH2 Modules

See Section 3.1 of Pruess et al. (1996) for a description of the predecessor codes from which TOUGH2 and the current items of discussion are derived.

#### 3.2 Structure and Architecture

##### Single-Phase Gas (EOS1G) and Saturated/Unsaturated (EOS9) Flow Modules

Following the TOUGH2 structure, the EOS1G and EOS9 TOUGH2 modules implement a flexible, general-purpose architecture (see Figure 3) for simulating fluid and heat flow in systems in which any number of components or species can be distributed among several coexisting phases. A key feature of the code architecture is a modular structure that allows for flexible interfacing between the module that sets up and solves the fluid flow equations and the EOS1G or EOS9 module, which represent fluid mixtures with different numbers of components and phases (see Table 1).

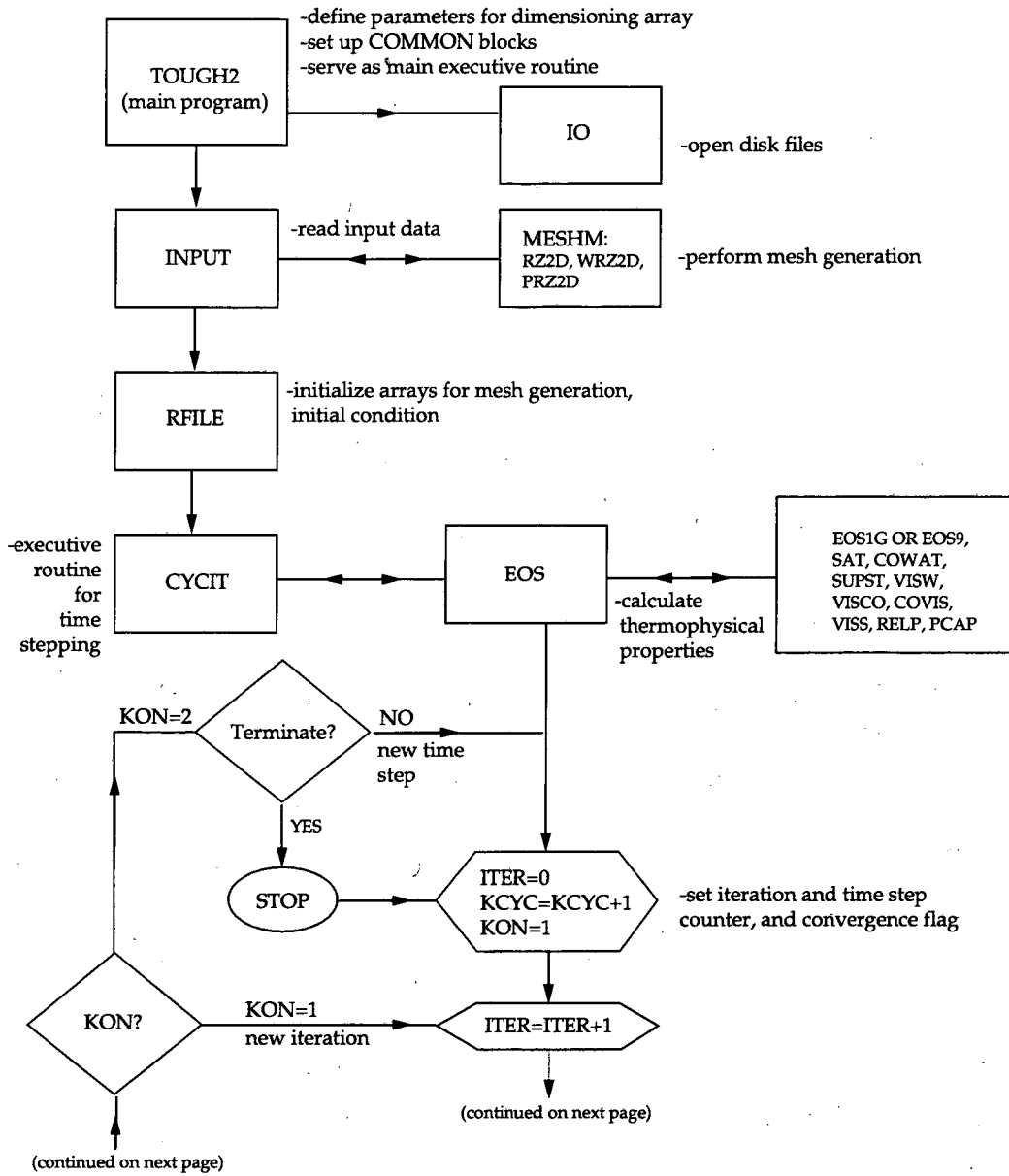
<u>Module</u>	<u>Capability</u>
EOS1G	gas (air and vapor) flow
EOS9	liquid (water and dissolved air) flow

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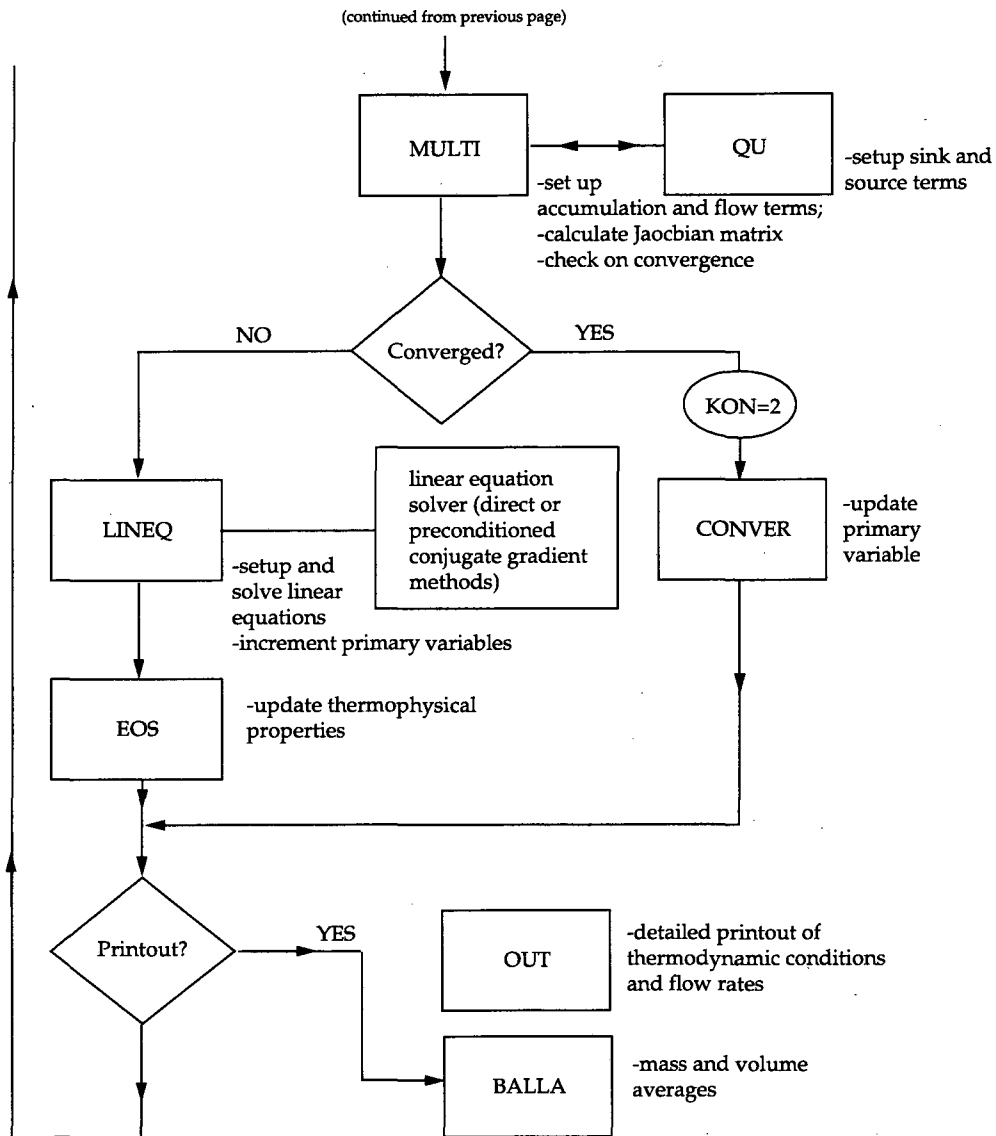
*Table 1. TOUGH2 single-phase gas and saturated/unsaturated flow module properties.*

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**Figure 3.** Structure of TOUGH2 single-phase gas (EOS1G) and saturated/unsaturated flow (EOS9) modules.



**Figure 3 (cont.).** Structure of TOUGH2 single-phase gas (EOS1G) and saturated/unsaturated flow (EOS9) modules.

User features include flexible dimensioning of major arrays, capabilities for internal processing of flow geometry through automatic mesh generation (via MESHMAKER), and enhanced abilities for specifying initial and boundary conditions. The input formats of the single-phase gas flow module follow those of TOUGH2 EOS3 module (see Pruess et al, 1996).

As in the standard TOUGH2 code, much of what program units do is spelled out in internal comments and in printed output in the gas flow module. In TOUGH2 the single-phase gas and saturated/unsaturated flow modules also provide a tight version control system for meeting stringent demands on reliability and referenceability of code applications. Each program unit, when first called during a TOUGH2 simulation run, writes a one-line message specifying its name, version number and date, and purpose. All version messages are optionally printed to OUTPUT at the end of a simulation run. An example of an OUTPUT file for the end of a run is shown in Figure 4. This lists all of the program units used in the simulation, their version number and date, and what they do. For the saturated/unsaturated flow module, the program units are similar to those of the TOUGH2 EOS3 module (Pruess et al., 1996), and are not listed here. Users who wish to modify the code can therefore maintain an easily referenceable record of code changes and applications by updating version messages for each program unit they change for internal use. The coding complies with the ANSI X3.9-1978 (FORTRAN 77) standard.

#### Effective Continuum Method Formulation Module (ECM)

This topic is not applicable in general, because the ECM module is only a subroutine of TOUGH2. The ECM module can be used in any TOUGH2 module for treating fracture-matrix flow. What the ECM module provides is a composite relative permeability for flow calculations in the fracture and matrix system, and the function is used by the TOUGH2 EOS modules.

***** * SUMMARY OF EOS1G PROGRAM UNITS * *****			
UNIT	VERSION	DATE	COMMENTS
IO	1.0	15 APR 1991	OPEN FILES *VERS*, *MESH*, *INCON*, *GENER*, *SAVE*, *LINEQ*, AND *TABLE*
SECOND	1.0E	27 MAY 1993	SUBROUTINE FOR CPU TIMING FUNCTION
TOUGH2	1.11CG	28 JAN 1994	MAIN PROGRAM WITH PRECONDITIONED CONJUGATE GRADIENT SOLVERS SPECIAL VERSION FOR PCS, 32-BIT WORD LENGTH
INPUT	1.02	30 JUN 1995	READ ALL DATA PROVIDED THROUGH FILE *INPUT*
FLOP	1.0	11 APR 1991	CALCULATE NUMBER OF SIGNIFICANT DIGITS FOR FLOATING POINT ARITHMETIC
RFILE	1.01	4 FEB 1993	INITIALIZE DATA FROM FILES *MESH* OR *MINC*, *GENER*, AND *INCON*
CYCIT	1.01	4 JAN 1995	EXECUTIVE ROUTINE FOR MARCHING IN TIME
PCAPGEN	1.0	14 JAN 1996	ECM CAPILLARY PRESSURE TABLE AS FUNCTION OF SATURATION
EOS1G	1.0	20 MAR 1996	*EOS1G* THERMOPHYSICAL PROPERTIES MODULE FOR SINGLE-PHASE AIR
SAT	1.0	22 JAN 1990	STEAM TABLE EQUATION: SATURATION PRESSURE AS FUNCTION OF TEMPERATURE
COWAT	1.0	22 JAN 1990	LIQUID WATER DENSITY AND INT. ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE
SUPST	1.0	29 JAN 1990	VAPOR DENSITY AND INTERNAL ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE
VISW	1.0	22 JAN 1990	VISCOSITY OF LIQUID WATER AS FUNCTION OF TEMPERATURE AND PRESSURE
VISCO	1.0	1 FEB 1990	CALCULATE VISCOSITY OF VAPOR-AIR MIXTURES
COVIS	1.0	1 FEB 1990	COEFFICIENT FOR GAS PHASE VISCOSITY CALCULATION
VISS	1.0	22 JAN 1990	VISCOSITY OF VAPOR AS FUNCTION OF TEMPERATURE AND PRESSURE
RELP	1.2	15 JAN 1996	LIQUID AND GAS PHASE RELATIVE PERMEABILITIES AS FUNCTIONS OF SATURATION
PCAP	2.0	15 JAN 1996	CAPILLARY PRESSURE AS FUNCTION OF SATURATION
RELP	1.0	25 JAN 1990	LIQUID AND GAS PHASE RELATIVE PERMEABILITIES AS FUNCTIONS OF SATURATION
BALLA	1.0	5 MAR 1991	PERFORM SUMMARY BALANCES FOR VOLUME, MASS, AND ENERGY
TSTEP	1.0	4 MAR 1991	ADJUST TIME STEPS TO COINCIDE WITH USER-DEFINED TARGET TIMES
MULTI	1.0	21 MAR 1996	ASSEMBLE ALL ACCUMULATION AND FLOW TERMS FOR 1-PH GAS FLOW
LINEQ	1.01 CG	27 NOV 1995	INTERFACE FOR LINEAR EQUATION SOLVERS
CONVER	1.1	1 DEC 1995	UPDATE PRIMARY VARIABLES AFTER CONVERGENCE IS ACHIEVED
WRIFI	1.0	22 JAN 1990	AT THE COMPLETION OF A TOUGH2 RUN, WRITE PRIMARY VARIABLES ON FILE *SAVE*
OUT	1.0	5 MAR 1991	PRINT RESULTS FOR ELEMENTS, CONNECTIONS, AND SINKS/SOURCES

*Figure 4, cont. Summary of single-phase gas module program units and version history.*

### Radionuclide Transport Module (T2R3D)

T2R3D follows the same general-purpose architecture of TOUGH2 (see Figure 5) for simulating fluid and heat flow and radionuclide transport in a geological system. As shown in Figure 5, the main difference from the TOUGH2 architecture is two additional subroutines for evaluating the hydraulic dispersion tensor and the radionuclide concentration gradients. Also, a new equation-of-state (EOSR3D) module is incorporated to represent fluid mixtures with three components and two phases (see Table 2). This new EOS module is based on the EOS3 module of TOUGH2.

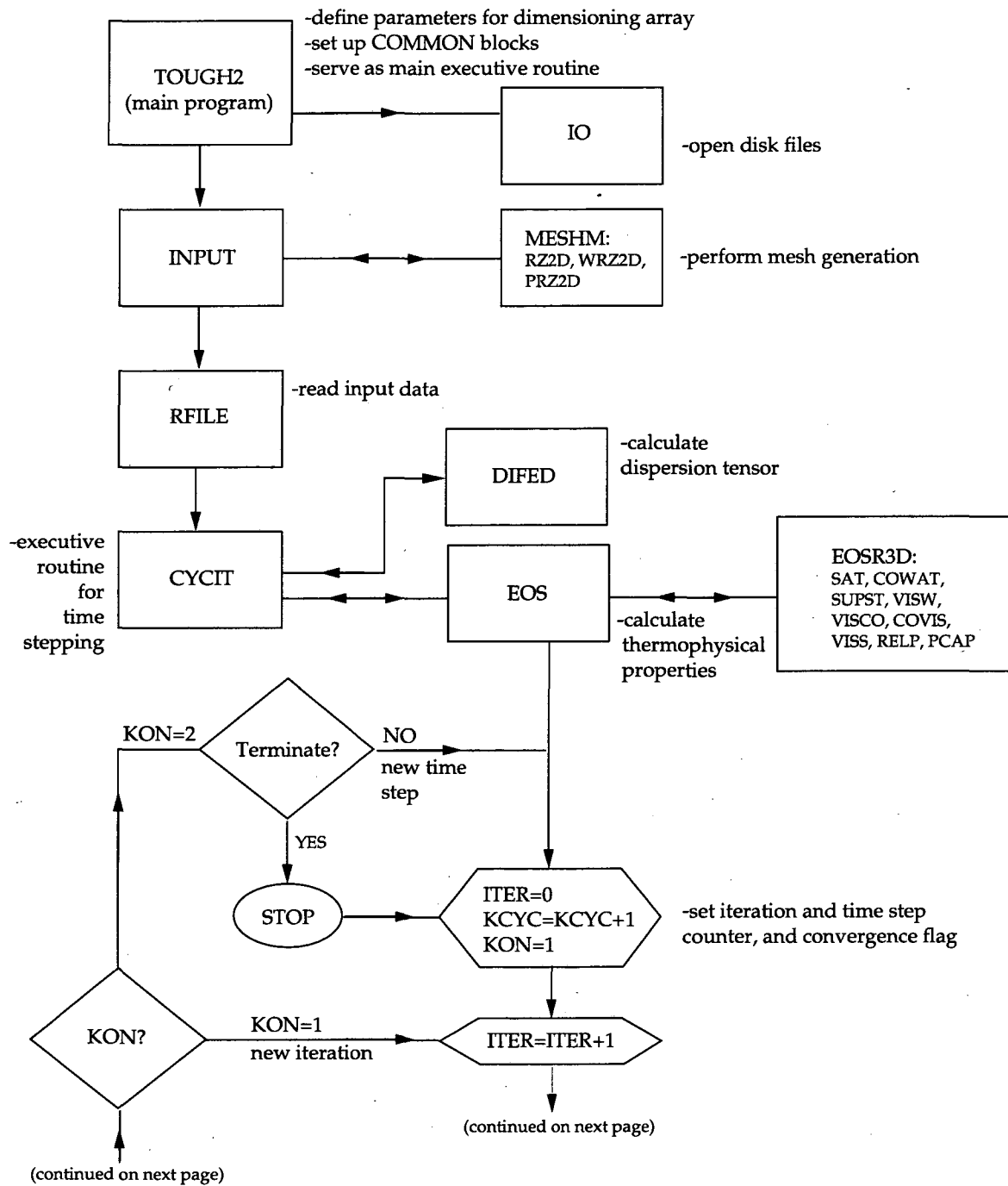


Figure 5. Structure of T2R3D: TOUGH2 radionuclide transport module.

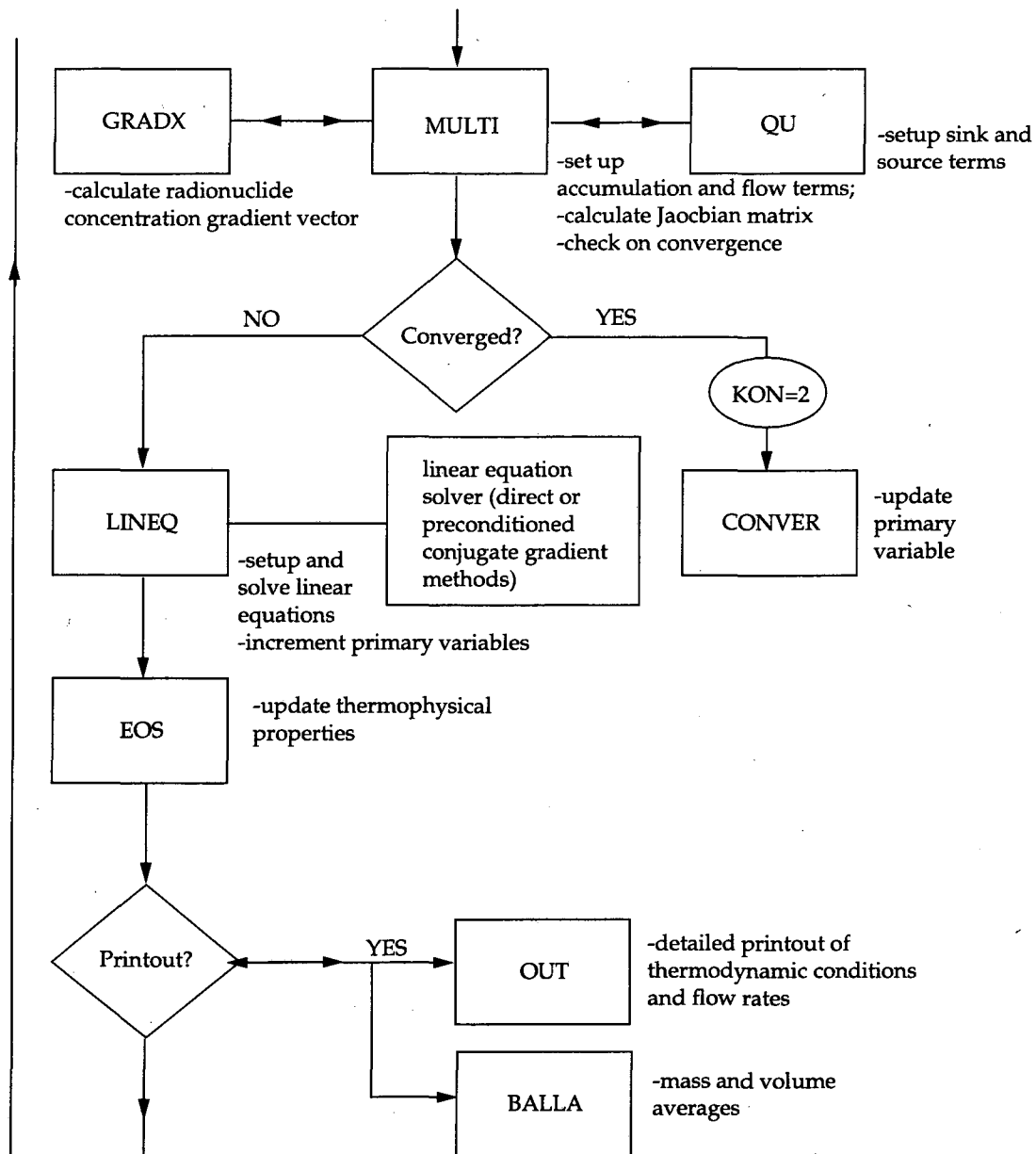


Figure 5, cont. Structure of TOUGH2 radionuclide transport module.

Module	Capability
T2R3D	Liquid, gas (air and vapor) and radionuclide (or tracer)

Table 2. TOUGH2 Fluid Property Module for Two-Phase Flow and Radionuclide Transport

User features of T2R3D are the same as those of TOUGH2, including internal capability of automatic mesh generation, and initial and boundary condition specifications. The input and output

formats of T2R3D follow those of the TOUGH2 EOS3 module, but the input data of T2R3D contain radionuclide transport properties in an additional line of ROCKS parameters. Also, the output of T2R3D includes the mass fraction of the radionuclide in the liquid phase, in addition to all of the information from the TOUGH2 EOS3 module.

Similar to the version control system for the standard TOUGH2, T2R3D provides a one-line message specifying its name, version number and date, and purpose of each subroutine. An example of a version control output at the end of a run is shown in Figure 6. This lists all of the program units called during the simulation, their version number and date, and functions. The coding of T2R3D complies with the ANSI X3.9-1978 (FORTRAN 77) standard.

***** * SUMMARY OF T2R3D PROGRAM UNITS * *****			
UNIT	VERSION	DATE	COMMENTS
IO WAZZU	1.0	15 APR 1991	OPEN FILES *VERS*, *MESH*, *INCON*, *GENER*, *SAVE*, *LINEQ*, AND *TABLE*
SECOND	1.0E	27 MAY 1993	SUBROUTINE FOR CPU TIMING FUNCTION
TOUGH2	1.11 CG	28 JAN 1994	MAIN PROGRAM WITH PRECONDITIONED CONJUGATE GRADIENT SOLVERS
INPUT	1.02	30 JUN 1995	READ ALL DATA PROVIDED THROUGH FILE *INPUT*
FLOP	1.0	11 APR 1991	CALCULATE NUMBER OF SIG. DIGITS FOR FLOATING POINT ARITHMETIC
RFILE	2.00	20 DEC 1995	INITIALIZE DATA FROM FILES *MESH* OR *MINC*, *GENER*, AND *INCON*
CYCIT	1.01	4 JAN 1995	EXECUTIVE ROUTINE FOR MARCHING IN TIME
CORDER	1.00	19 DEC 1995	SORT THE INDEX OF TOTAL CONNECTIONS FOR EACH BLOCK
EOSR3D	3.0	11 DEC 1995	*EOSR3D* THERMOPHYSICAL PROPERTIES MODULE FOR WATER/AIR
SAT	1.0	22 JAN 1990	STEAM TABLE EQUATION: SATURATION PRESSURE AS FUNC. OF TEMP.
VISW	1.0	22 JAN 1990	VISCOSITY OF LIQUID WATER AS FUNCTION OF TEMPERATURE AND PRESSURE
COWAT	1.0	22 JAN 1990	LIQUID WATER DENSITY AND INT. ENERGY AS FUNC. OF TEMP. AND PRESSURE
PCAP	2.0	15 JAN 1996	CAPILLARY PRESSURE AS FUNCTION OF SATURATION
BALLA	1.0	5 MAR 1991	PERFORM SUMMARY BALANCES FOR VOLUME, MASS, AND ENERGY
DIFFD	1.00	19 DEC 1995	CALCULATE DIFFUSIVE TENSOR
TSTEP	1.0	4 MAR 1991	ADJUST TIME STEPS TO COINCIDE WITH USER-DEFINED TARGET TIMES
MULTI	2.0	11 DEC 1995	ASSEMBLE ALL ACCUMULATION AND FLOW TERMS
SUPST	1.0	29 JAN 1990	VAPOR DENSITY AND INTERNAL ENERGY AS FUNC. OF TEMP. AND PRESSURE
GRADX	1.00	19 DEC 1995	CALCULATE CONCENTRATION GRAD VECTOR
LINEQ	1.01 CG	27 NOV 1995	INTERFACE FOR LINEAR EQUATION SOLVERS
CONVER	1.1	1 DEC 1995	UPDATE PRIMARY VARIABLES AFTER CONVERGENCE IS ACHIEVED

Figure 6. Summary of radionuclide transport module program units and version history.

### 3.3 Physical Processes and Approximations

#### 3.3.1 Single-Phase Gas (EOS1G) and Saturated/Unsaturated (EOS9) Flow Modules

The TOUGH2 simulator takes account of the following physical processes with the governing equations provided in Appendix A of Pruess et al. (1996). Fluid flow in both gaseous (EOS1G) and liquid (EOS9) phases occurs under pressure, viscous, and gravity forces according to Darcy's law, with interference between the phases represented by means of relative permeability functions. Mass-balance equations are written in integral form for an arbitrary flow domain. In addition, the single-phase gas formulation accounts for a simplified description of Knudsen diffusion by means of a Klinkenberg factor for permeability (Knudsen, 1909; Klinkenberg, 1941;



Hadley, 1982). Capillary pressure effects are taken into account for the liquid phase in the EOS9 module.

The transport equations are complemented with constitutive relationships, which express all parameters as functions of a set of thermodynamic variables. All thermophysical properties of liquid water and vapor are obtained within experimental accuracy from steam table equations (International Formulation Committee, 1967). In EOS1G, air is treated as an ideal gas, and additivity of partial pressures is assumed for air/vapor mixtures. The viscosity of air/vapor mixtures is computed from a formulation given by Hirschfelder et al. (1954), using steam table values for vapor viscosity.

In EOS1G, liquid water and heat are assumed to be at steady-state, but could be non-uniformly distributed within the system considered. In EOS9, temperature and gas pressure are assumed to be uniformly distributed within the system considered. The description of thermodynamic conditions is based on assumed local equilibrium of all phases.

The governing equations used in the TOUGH2 single-phase gas flow module and the saturated/unsaturated flow module and their numerical implementation are applicable to one-, two-, or three-dimensional anisotropic porous or fractured media. As in standard TOUGH2, these modules do not allow for deformation of the host medium and its effects on the multiphase flow behavior, but allow for porosity changes in response to changes in pore pressure (compressibility) and temperature (expansivity).

### 3.3.2 Effective Continuum Method Formulation Module (ECM)

The ECM formulation is based on a single key assumption that there be approximate thermodynamic equilibrium (locally) between fracture and matrix at all times (Pruess et al., 1988). If we consider single-component, two-phase flow in a fractured porous medium, the conditions for thermodynamic equilibrium are:

- (1) equality of temperatures

$$T_m \cong T_f \quad (3.3.2.1)$$

and

- (2) equality of pressures

$$P_{\beta,m} \cong P_{\beta,f} \quad (\beta = \text{liquid, gas}) \quad (3.3.2.2)$$

Under such a condition, we will have equality of capillary pressures:

$$P_{c,m} \cong P_{c,f} \quad (3.3.2.3)$$

and equality of fluid density

$$\rho_{\beta,m} \cong \rho_{\beta,f} \quad (3.3.2.4)$$

and viscosities:

$$\mu_{\beta,m} \cong \mu_{\beta,f} \quad (3.3.2.5)$$

### 3.3.3 Radionuclide Transport Module (T2R3D)

T2R3D is a computer code for multiphase fluid and heat flow, and radionuclide transport in permeable geological media. It takes account of the physical processes of a radionuclide or tracer transport in a non-isothermal multi-phase flow environment in the subsurface. The treatment of water, gas and heat flow is identical to that of the TOUGH2 EOS3 module (Pruess, 1991). The major assumptions for the radionuclide transport module are (a) a radionuclide or a tracer exists and is transported only within the liquid phase, (b) radionuclide transport mechanisms include molecular diffusion and hydraulic dispersion in the liquid phase in addition to advection, (c) first order decay is taken into account, and (d) adsorption of radionuclides on the rock matrix is described by an equilibrium isotherm with a constant distribution coefficient. The radionuclide or tracer is introduced as an additional mass component into the standard TOUGH2 formulation.

## 3.4 Mathematical and Numerical Methods

### 3.4.1 Single-Phase Gas (EOS1G) and Saturated/Unsaturated (EOS9) Flow Modules

Continuum equations for mass-balance of the air component for the single-phase gas module, and the water component for the saturated/unsaturated flow module, are discretized in space using the "integral finite difference" method (Edwards, 1972; Narasimhan and Witherspoon, 1976). See Appendix A and Appendix B for details of these methodologies. Introducing appropriate volume averages, we have

$$\int_{V_n} M dv = V_n M_n \quad (3.4.1.1)$$

Here  $M$  is a volume-normalized extensive quantity, and  $M_n$  is the average value of  $M$  over  $V_n$ . Surface integrals are approximated as a discrete sum of averages over surface segments. Time is discretized fully implicitly as a first order finite difference to obtain the numerical stability needed for an efficient calculation of multi-phase flow. In the process of matrix formulation, various degrees of upstream weighting may be chosen. For each volume element (grid block or  $N$ ), either the gas phase pressure in EOS1G and the liquid pressure (saturated) or liquid saturation (unsaturated) in EOS9 are chosen as the primary variable to define the thermodynamic state of the flow system. A space and time discretization yields a coupled set of algebraic equations (see Pruess, 1987). The total number of mass-balance equations is equal to the number of primary variables times the number of grid blocks. The equations are still coupled because of interdependence of gas or liquid flow. They are non-linear in EOS1G because of high compressibility of the gas phase, and also in EOS9 because of non-linear material properties such as relative permeability and capillary pressure. Because of these features of the equation system, TOUGH2 performs a simultaneous solution of the discretized mass-balance equations, taking all coupling terms into account. Non-linearities are handled by performing the Newton/Raphson iteration. The unknowns are the  $N$  independent "primary" variables, which completely define the thermodynamic state of the flow system at time level  $t^{k+1}$ . See Table 3.

<u>Phase Composition</u>	<u>Primary Variable</u>
single-phase gas	P - gas pressure
saturated/unsaturated flow	$S_w$ - liquid saturation, for two-phase conditions P - water pressure, for single-phase liquid conditions

Table 3. Primary Thermodynamic Variables

Upon application of the Newton/Raphson iteration (see Pruess, 1987), a set of N coupled linear equations is obtained. These can be solved with an iterative sparse matrix solver (Forsyth, 1992). Iteration is continued until the residuals are reduced to a small fraction of the accumulation terms. See Pruess (1987) for convergence criteria. Convergence is usually obtained in three to four iterations. If convergence cannot be achieved within a certain number of iterations, the time step size  $\Delta t$  is reduced and a new iteration process is started. All derivatives needed in the coefficient matrix are obtained by numerical differentiation. The resulting Jacobian matrix is solved to yield the changes in the primary variables in each element of the discretized domain from the previous iteration.

The entire geometric information of the space discretization is provided in the form of a list of grid block volumes, interface areas, nodal distances, and components of gravitational acceleration along nodal lines. The discretized equations are valid for arbitrary irregular discretizations in one, two, or three dimensions, and for porous as well as for fractured media. This flexibility should be used with caution, however, because the accuracy of solutions depends upon the accuracy with which the various interface parameters can be expressed in terms of average conditions in grid blocks (see Pruess, 1987). A necessary condition for this is approximate thermodynamic equilibrium in almost all grid blocks at almost all times (Pruess and Narasimhan, 1985). For systems of regular grid blocks referenced to global coordinates, the equations reduce to a conventional finite difference formulation (Peaceman, 1977).

### 3.4.2 Effective Continuum Method Formulation Module (ECM)

Darcy's law for single-component two-phase flow in a fractured porous medium can be written in the following form.

$$\mathbf{F}_{\beta, \text{matrix}} = -k_m k_{\beta, m} \left( \frac{\rho_{\beta}}{\mu_{\beta}} \right)_m (\nabla P_{\beta, m} - \rho_{\beta, m} \mathbf{g}) \quad (3.4.2.1)$$

$$\mathbf{F}_{\beta, \text{fractures}} = -k_f k_{\beta, f} \left( \frac{\rho_{\beta}}{\mu_{\beta}} \right)_f (\nabla P_{\beta, f} - \rho_{\beta, f} \mathbf{g}) \quad (3.4.2.2)$$

The notation for equations (3.3.2.1) through (3.4.2.9) is as follows:

- $\mathbf{F}$  = mass flux
- subscript  $\beta$  = phase index ( $\beta$ =liquid, gas)
- subscript m = relating to matrix
- subscript f = relating to fractures
- subscript c = relating to capillary pressure
- subscript  $\ell$  = relating to liquid
- $k_m$  ( $k_f$ ) = equivalent single-phase continuum permeability, or permeability tensor for an anisotropic system of matrix (fractures)
- $k_{\beta, m}$  ( $k_{\beta, f}$ ) = relative permeability to phase  $\beta$  in matrix (fractures),
- $\rho_{\beta}$  = density of phase  $\beta$
- $\mu_{\beta}$  = viscosity of phase  $\beta$
- $P_{\beta}$  = pressure of phase  $\beta$

$\mathbf{g}$  = acceleration of gravity  
 $s$  = liquid saturation

Under conditions of (local) thermodynamic equilibrium we have the following expression for total flux (note that equality of pressures implies equality of pressure gradients):

$$\begin{aligned} \mathbf{F}_\beta &= \mathbf{F}_{\beta, \text{matrix}} + \mathbf{F}_{\beta, \text{fracture}} \\ &= -\left(k_m k_{\beta, m} + k_f k_{\beta, f}\right) \frac{\rho_\beta}{\mu_\beta} (\nabla P_\beta - \rho_\beta \mathbf{g}) \end{aligned} \quad (3.4.2.3)$$

Here, the relative permeabilities  $k_{\beta, m}$  and  $k_{\beta, f}$  have to be evaluated at saturations  $S_{\beta, m}$  and  $S_{\beta, f}$  respectively, such that

$$P_{c, m}(S_{\beta, m}) = P_{c, f}(S_{\beta, f}) \quad (3.4.2.4)$$

The expression for total flux can be interpreted as referring to a single effective continuum with total effective phase permeability of  $k_m k_{\beta, m} + k_f k_{\beta, f}$ . For single-phase flow, the effective continuum permeability becomes  $k = k_m + k_f$ , so that the effective continuum relative permeability can be defined as

$$k_\beta = \frac{k_m k_{\beta, m} + k_f k_{\beta, f}}{k_m + k_f} \quad (3.4.2.5)$$

The total phase flux is then given by the following single continuum expression

$$\mathbf{F}_\beta = -k_\beta \frac{\rho_\beta}{\mu_\beta} (\nabla P_\beta - \rho_\beta \mathbf{g}) \quad (3.4.2.6)$$

In these equations we have defined relative permeabilities relative to total single-phase permeability, so that  $0 < k_\beta < 1$ .

The numerical implementation of the ECM scheme for evaluating the effective continuum permeabilities is straightforward once we know liquid saturations in matrix and fracture, respectively. This can be achieved by introducing a fracture/matrix combined (or composite) capillary pressure ( $P_c$ ) curve, based on the individual fracture and matrix  $P_c$  curves from input. Under local equilibrium conditions, the combined  $P_c$  curve is

$$P_c(S_\ell) = P_{c, m}(S_{\ell, m}) = P_{c, f}(S_{\ell, f}) \quad (3.4.2.7)$$

as a function of a combined or average liquid saturation:

$$S_\ell = \frac{S_{\ell, m} \phi_m + S_{\ell, f} \phi_f}{\phi_m + \phi_f} \quad (3.4.2.8)$$

Then, during the Newton/Raphson iteration in the TOUGH2 solution, the obtained liquid saturation from the solver is exactly the combined saturation. The saturation value can be used in the combined  $P_c$  curve to calculate the value of the combined capillary function, which is the same as that of fracture or matrix systems. The fracture and matrix saturations can then be determined

by inverting the  $P_c$  functions of fracture and matrix, respectively. The ECM relative permeabilities are evaluated as follows:

$$k_{rel}^i = \frac{k_m^i k_{\ell,m}(S_{\ell,m}) + k_f^i k_{\ell,f}(S_{\ell,f})}{k_m^i + k_f^i} \quad (3.4.2.9)$$

Where the superscript  $i$  denotes the permeability in a principal direction ( $i=1, 2, \text{ and } 3$ ) to account for anisotropic properties of permeabilities in the fractures and matrix, respectively.

### 3.4.3 Radionuclide Transport Module (T2R3D)

The basic mass and thermal energy balance equations solved by T2R3D are the same in form as those by the standard TOUGH2 EOS3 module (Pruess et al., 1996). The only difference is that T2R3D introduces an additional component, a radionuclide. Therefore, the total number of components in T2R3D is three, with component #1 = water, #2 = air, and #3 = radionuclide. The numerical scheme used in T2R3D is identical with that of the TOUGH2 code, and is based on the integral finite different scheme. Time is discretized fully implicitly, and non-linearities are handled using Newton/Raphson iteration.

The mass balances for water, air and radionuclide components are described by Equations (B.1) and (B.2) (see Appendix B) with component index  $\kappa = 1, 2 \text{ and } 3$  for water, air and radionuclide, respectively. The equations for liquid, gas and heat flow are handled in the same way as in the TOUGH2 code (Pruess, 1991). However, the mass flux term for the radionuclide in the liquid phase is described by

$$\mathbf{F}^{(\kappa)} = \mathbf{F}_A^{(\kappa)} + \mathbf{F}_D^{(\kappa)} \quad (3.4.3.1)$$

where  $\kappa = 3$  for the radionuclide component. In Equation (3.4.3.1), the first term on the right-hand side is mass flux by advection, defined as

$$\mathbf{F}_A^{(\kappa)} = X_\beta^{(\kappa)} \mathbf{F}_\beta \quad (3.4.3.2)$$

where the phase flux  $\mathbf{F}_\beta$  ( $\beta = \text{liquid}$ ) is given in Equation (A.4) by Darcy's law, and  $X_\beta^{(\kappa)}$  is the mass fraction of radionuclide in the liquid phase.

The second term on the right-hand side of (3.4.3.1) is the dispersive and diffusive mass flux, defined as

$$\mathbf{F}_D^{(\kappa)} = -\rho_\beta \bar{\mathbf{D}} \cdot \nabla X_\beta^{(\kappa)} \quad (\beta=\text{liquid}, \kappa=3) \quad (3.4.3.3)$$

where  $\bar{\mathbf{D}}$  is the combined diffusion-dispersion tensor accounting for both molecular diffusion and hydraulic dispersion. We have incorporated a general dispersion model for 3-D radionuclide transport into the T2R3D code (Scheidegger, 1961),

$$\bar{\mathbf{D}} = \alpha_T |\mathbf{v}_\beta| \delta_{ij} + (\alpha_L - \alpha_T) \frac{\mathbf{v}_\beta \mathbf{v}_\beta}{|\mathbf{v}_\beta|} + \phi S_\beta \tau d_m \delta_{ij} \quad (\beta=\text{liquid}) \quad (3.4.3.4)$$

where  $\alpha_T$  and  $\alpha_L$  are the transverse and longitudinal dispersivities, respectively;  $v_\beta$  is the Darcy's velocity vector of phase  $\beta$ ;  $\tau$  is the tortuosity of the medium;  $d_m$  is the molecular diffusion coefficient in phase  $\beta$ ; and  $\delta_{ij}$  is the Kroneker delta function. ( $\delta_{ij}=1$  for  $i=j$ , and  $\delta_{ij}=0$  for  $i \neq j$ )

The treatment of adsorption and first-order decay effects in T2R3D follows the work by Oldenburg and Pruess (1995, EOS7R) using the integral finite difference formulation. The mass accumulation term including adsorbed radionuclide on the rock matrix is

$$M^{(\kappa)} = \phi S_\beta \rho_\beta X_\beta^{(\kappa)} + (1 - \phi) \rho_R \rho_\beta X_\beta^{(\kappa)} K_d \quad (3.4.3.5)$$

where  $\rho_R$  is the rock matrix density and  $K_d$  is the distribution coefficient of the radionuclide partitioning between the aqueous phase and rock grains.

The first-order decay of a radionuclide is handled by the discretized equation (Oldenburg and Pruess, 1995),

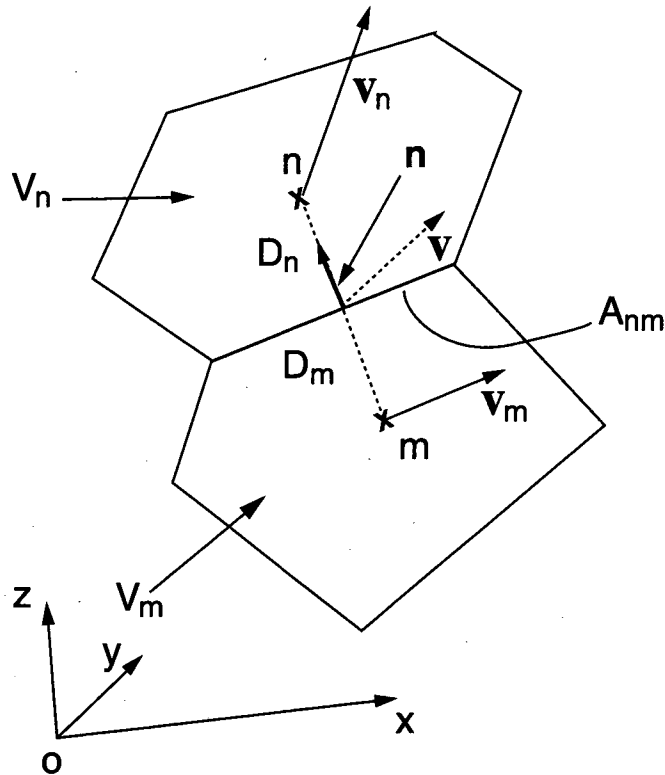
$$M_n^{k,k+1} (1 + \lambda_\kappa \Delta t) - M_n^{k,k} = \frac{\Delta t}{V_n} \left\{ \sum_m A_{nm} F_{nm}^{k,k+1} + V_n q_n^{k,k+1} \right\} \quad (3.4.3.6)$$

where  $\lambda_\kappa$  is the radioactive decay constant of the radionuclide (component  $\kappa=3$ ), and is defined as

$$\lambda_\kappa = \frac{\ln(2)}{T_{1/2}} \quad (3.4.3.7)$$

and  $T_{1/2}$  is the half-life of the radionuclide component.

One of the key issues in implementing the general 3-D dispersion tensor of (3.4.3.4) into T2R3D is how to average velocity fields for determining the dispersion tensor. We have adopted a spatial and harmonic weighting scheme to evaluate a velocity vector at the interfaces between element blocks, as shown in Figure 7.



**Figure 7.** Schematic of spatial averaging scheme for velocity fields in the integral finite difference method

In Figure 7,  $V_m$  and  $V_n$  are the volumes of blocks  $m$  and  $n$ ,  $A_{nm}$  is the area of the interface between the two blocks,  $D_m$  and  $D_n$  are the distances from the interface to each block's center, and  $v_m$  and  $v_n$  are the fluid velocities at the center of each block, while  $v$  is the velocity of liquid at the interface between blocks.  $n$  is the unit vector at the connection between the two blocks along connection  $nm$ , with a component  $n_i$  ( $i=x,y,z$ ), or directional cosines, in the  $x$ -,  $y$ -, or  $z$ -direction, respectively. Also the positive direction of  $n$  is defined as the direction from the block center of  $V_m$  toward the block center of  $V_n$ , as shown in Figure 7.

All three velocity vectors,  $v_n$ ,  $v_m$ , and  $v$ , and the connection-direction vector,  $n$ , are relative to the global coordinate system of  $(x, y, z)$ , as shown in Figure 7.

First we need to convert the local fluxes along connections in the local coordinates to a velocity vector,  $v_n$ , in the system of global coordinates  $(x, y, z)$  at the block center for each block of the grid. The averaging or weighting scheme used is called "**projected area weighting method**", and in this method a velocity component,  $v_{n,i}$ , of the vector  $v_n$  is determined by the vectorial summation of the components of all local connection vectors in the same direction, weighted by the projected area in that direction,

$$v_{n,i} = \frac{\sum_m (A_{nm} |n_i|) (v_{nm} n_i)}{\sum_m (A_{nm} |n_i|)} \quad (3.4.3.8)$$

( $i=x,y,z$ )

where  $m$  is the total number of connections between element  $V_n$  and all its neighboring elements  $V_m$ , and  $v_{nm}$  is the flux along connection  $nm$  in the local coordinate system. In Equation (3.4.3.8), the term,  $(A_{nm}|n_i|)$ , is the projected area of the interface  $A_{nm}$  on to the direction  $i$  of the global coordinate system, and  $(v_{nm}n_i)$  gives the velocity component in the direction  $i$  of the global coordinate system, contributed by the local flux  $v_{nm}$  between blocks  $V_n$  and  $V_m$ . Also it should be mentioned that the absolute value for the directional cosines,  $n_i$ , are used for evaluating the projected area in Equation (3.4.3.8), because only the positive areal values are needed for the weighting scheme.

The velocity vector  $v$  at the interface of elements  $n$  and  $m$  is evaluated by harmonic weighting by the distances to the interface using the velocities at the block centers of the two elements,

$$\frac{D_n + D_m}{V_i} = \frac{D_n}{V_{n,i}} + \frac{D_m}{V_{m,i}} \quad (i=x, y, z) \quad (3.4.3.9)$$

for its component  $v_i$ . Harmonic weighting is used because it preserves total transit time for solute transport.

The velocity  $v$  or  $v_\beta$ , determined by equation (3.4.3.9), is used in Equation (3.4.3.4) to evaluate the dispersion tensor along the connection of the two elements.

The concentration or mass fraction gradient of the radionuclide is evaluated, based on the "*interface area weighting scheme*". The mass fraction gradient, a vector, at element  $n$  is given by an areal weighting scheme:

$$\nabla X_n^{(\kappa)} = \frac{\sum_m A_{nm} \nabla X_{nm}^{(\kappa)}}{\sum_m A_{nm}} \quad (\kappa=3) \quad (3.4.3.10)$$

where  $\nabla X_{nm}^{(\kappa)}$  is the mass fraction gradient of a radionuclide along connection  $nm$  in the global coordinate system,

$$\nabla X_{nm}^{(\kappa)} = (n_x \Delta X_{nm}^{(\kappa)}, n_y \Delta X_{nm}^{(\kappa)}, n_z \Delta X_{nm}^{(\kappa)}) \quad (3.4.3.11)$$

and

$$\Delta X_{nm}^{(\kappa)} = \frac{X_m^{(\kappa)} - X_n^{(\kappa)}}{D_m + D_n} \quad (3.4.3.12)$$

The reason behind the interface area weighting method is that the dispersive fluxes between all the connected elements are directly proportional to the interface areas, therefore a local concentration gradient with a larger connected interface area should take more weight in the resultant gradient at the block.

The mass fraction gradient  $\nabla X$  at the interface between two blocks is evaluated by a linear interpolation for its component  $i$  ( $i=x, y, z$ ),



$$\nabla X_i^{(\kappa)} = \frac{D_m}{D_m + D_n} \nabla X_{n,i}^{(\kappa)} + \frac{D_n}{D_m + D_n} \nabla X_{m,i}^{(\kappa)} \quad (3.4.3.13)$$

This mass fraction gradient of (3.4.3.13) will be used to calculate the total diffusive and dispersive mass flux of a radionuclide along the connection of the two elements.

The net mass flux of diffusion and dispersion of a radionuclide along the connection of elements  $V_n$  and  $V_m$  is determined by

$$F_{nm}^{(\kappa)} = \mathbf{n} \cdot \mathbf{F}_D^{(\kappa)} = -\mathbf{n} \cdot \left[ \rho_\beta \bar{D} \cdot \nabla X_\beta^{(\kappa)} \right] \quad (3.4.3.14)$$

Finally, the diffusive and dispersive flux of equation (3.4.3.14) is added to the total flux term of a radionuclide along the connection of the two elements in the MULTI subroutine of T2R3D.

### 3.5 Array Structure and Handling

#### Single-Phase Gas (EOS1G), Saturated/Unsaturated Flow (EOS9), and Radionuclide Transport (T2R3D) Modules

The number of primary thermodynamic variables that is needed to completely specify the thermodynamic state of a flow system is  $NEQ=1$  for the single-phase gas and saturated/unsaturated flow modules. For the radionuclide transport module, the primary variable number is  $NEQ=4$ . The thermodynamic state of a discretized flow system containing  $NEL$  (number of elements) volume elements or grid blocks is then completely specified by a set of  $NEL*NEQ$  primary thermodynamic variables, to which correspond an equal number of air or water mass equations. For transient flow systems, these primary variables are time-dependent, and they represent the unknowns to be calculated in each time step. In the TOUGH2 single-phase gas flow, saturated/unsaturated flow, and radionuclide transport modules, all of the  $NEL*NEQ$  variables are stored sequentially in a one-dimensional array  $X$  as in TOUGH2.

There are two additional arrays  $DX$  and  $DELX$  with structure identical to  $X$ . While  $X$  holds the primary variables corresponding to the last successful (converged) time step,  $DX$  holds the latest increments calculated during the Newton/Raphson iteration process. Thus the latest updated primary variables are the quantities  $X+DX$ . The array  $DELX$  holds small increments of the  $X$  themselves (typically on the order  $10^{-7}*X$ ) which are used to calculate incremented parameters needed for the numerical calculation of the derivatives in the Jacobian matrix  $J = -\partial \mathbf{R}_n / \partial \mathbf{X}_i$ . At the conclusion of a converged time step, the primary variables  $X$  are updated,  $X \rightarrow X+DX$ .

The fluid property modules calculate all thermophysical properties (secondary parameters) needed to assemble the air or water mass-balance equations for the latest updated primary variables  $X+DX$ . These parameters are then stored sequentially in a large array  $PAR$ . The number of secondary parameters other than component mass fractions is  $NB$  (usually  $NB=8$  to include two anisotropic relative permeability functions); in addition there is one mass fraction each for EOS1G and EOS9, and three for T2R3D so that the total number of secondary parameters per fluid phase is  $NBK=NB+NK$ . The  $PAR$  array structure for EOS1G and EOS9 is the same as for the case of two fluid phases.

### 3.6 Linear Equation Setup

#### Single-Phase Gas (EOS1G), Saturated/Unsaturated Flow (EOS9), and Radionuclide Transport (T2R3D) Modules

The data provided by the PAR-array are used in these three modules of TOUGH2 to assemble the linear equations (Eq. B.7) that are solved at each step of the Newton/Raphson iteration procedure. These equations are arranged and numbered sequentially, with one equation per grid block representing air component mass balances for the single-phase gas flow module. Also, for the saturated/unsaturated flow module, one equation per grid block is set up for the water mass balances. There are four equations per grid block set up in T2R3D, for water, air, radionuclide components, and heat. The row indices of the Jacobian matrix correspond to the sequence of primary variables in array X.

Note that the accumulation terms of the balance equations depend only on primary variables for one grid block, so that they will generate non-zero derivative terms only in a 1x1 or 4x4 submatrix that is located on the diagonal of the Jacobian J. The flow terms, being dependent on primary variables of two grid blocks, will generate two non-zero 1x1 or 4x4 submatrices of derivatives, which are located in the off-diagonal matrix locations corresponding to the two grid blocks.

It should be noted that the dispersive fluxes evaluated for a radionuclide in T2R3D depend not only on the primary variables of the two connected grid blocks, but also on the primary variables in all the neighboring grid blocks, which are used to calculate the average velocity and concentration gradient vectors. This gives rise to additional terms in the Jacobian matrix relative to the standard TOUGH2 formulation, which, however, have been ignored in the T2R3D solution procedure. Therefore, the T2R3D actually uses an incomplete-Jacobian Newton/Raphson iteration scheme. This treatment will not affect the final solution as long as the convergence rate of a solution is obtained, which depends only on the residual equations. However, the convergence rate of a numerical solution may deteriorate in certain cases because a fully Jacobian matrix is not used.

As in the TOUGH2 code, in these three modules all Jacobian matrix elements as well as the entries in the vector R of residuals are calculated in subroutine "MULTI". The calculation first assigns all matrix elements arising from the accumulation terms, of which there are  $NEQ * NEQ$ . Calculation of the derivatives demands that each accumulation term is calculated  $NEQ + 1$  times; once for the state point  $(X + DX)$ , and  $NEQ$  times for each of the  $NEQ$  primary variables incremented  $(X + DX + DELX)$ . Additional contributions to diagonal terms in the Jacobian J may arise from sink and source terms if present; these are assigned in subroutine QU called from MULTI. Subsequently all flux terms are evaluated. These depend in general on the  $2 * NEQ$  primary variables of the two connected grid blocks, so that a total of  $2 * NEQ + 1$  flux terms need to be evaluated for calculation of the state point as well as of all derivative terms.

After all matrix elements and members of the right-hand side vector of residuals have been calculated, the package of iterative matrix solvers (Forsyth, 1992) is called to solve the linear equations (Eq. B.7). The resulting increments in the primary variables are added to the array DX, and the process of linear equation setup and solution is repeated for the primary variables  $X + DX$ . This process continues until the residuals are reduced below a preset convergence tolerance. If convergence is not achieved within a specified maximum number of iterations (usually eight), the time step is repeated with reduced time increment.

### 3.7 Dimensioning of Major Arrays

#### Single-Phase Gas (EOS1G), Saturated/Unsaturated Flow (EOS9), and Radionuclide Transport (T2R3D) Modules

The major problem-size dependent arrays reside in COMMON blocks, which are dimensioned by means of a PARAMETER statement in all subroutines of the TOUGH2 single-phase gas flow, saturated/unsaturated flow, and radionuclide transport programs. The user will specify the sizes of different arrays by modifying the INCLUDE parameter file "TOUGH2.PRM", and recompiling the codes.

### 3.8 Equation-of-State Modules

The thermophysical properties of fluid mixtures needed in assembling the governing mass-balance equations are provided by equation-of-state modules that provide values for all secondary (thermophysical) parameters as functions of the primary variables.

#### Single-Phase Gas Flow Module (EOS1G)

EOS1G (Air): This module is an adaptation of the EOS3 module of the TOUGH2 program, and implements the same thermophysical properties model (see Pruess, 1987). All water properties are represented by the steam table equations (International Formulation Committee, 1967). Air is approximated as an ideal gas, and additivity is assumed for air and vapor partial pressures in the gas phase,  $P_g = P_a + P_v$ . The viscosity of air-vapor mixtures is computed from a formulation given by Hirschfelder et al. (1954).

EOS1G differs from the EOS3 module of TOUGH2 in the following ways: (1) the primary thermodynamic variable is always gas pressure, (2) water phase is treated as a passive phase with stable distribution, and (3) temperature will not change. The system is assumed to be at two-phase conditions. Primary variables should be initialized identically to TOUGH2 (EOS3) specifications by setting  $MOP(19) = 0$ . A summary of EOS1G specifications is given in Table 4.

<b>COMPONENTS</b>	#1: air
<b>PARAMETER CHOICES</b>	
(NK, NEQ, NPH, NB) =	(1,1,1,8)
MOP(19) =	0
<b>PRIMARY VARIABLES</b>	
(P) - (gas phase pressure)	

*Table 4. Summary of EOS1G*

#### Saturated/Unsaturated Flow Module (EOS9)

EOS9 is a simplified version of EOS3 which provides all the thermophysical properties of the liquid phase needed in assembling the governing water mass balance equations. This module evaluates all secondary (thermophysical) parameters as functions of the primary variables. The primary variable is water saturation under two-phase conditions and water pressure for a single

liquid phase. Also in EOS9, liquid water properties are treated in the same way as in the TOUGH2 EOS3 module.

<b>COMPONENTS</b>	#1: water
<b>PARAMETER CHOICES</b>	
(NK, NEQ, NPH, NB) =	(1,1,1,8)
<b>PRIMARY VARIABLES</b>	
Single phase condition ( $P_w$ ) - (Water pressure)	
Two phase condition ( $S_w$ ) - Water saturation	

*Table 5. Summary of EOS9.*

### Radionuclide Transport Module (T2R3D)

The EOS module for the radionuclide transport program (T2R3D) is called EOSR3D, and it handles all the flow and transport properties for water, air, radionuclide, and heat under two-phase and non-isothermal conditions.

EOSR3D provides all the thermophysical properties of fluid mixtures needed in assembling the governing mass and thermal energy balance equations. This module evaluates all secondary (thermophysical) parameters as functions of the primary variables.

EOSR3D (Water, Air, Radionuclide and Heat): This module is a modified version of the EOS3 module of the TOUGH2 program (See Pruess, 1991). All water, gas and thermal properties are treated in the same way as in TOUGH2. EOSR3D treats the radionuclide as a liquid tracer which does not affect liquid properties, and radionuclide mass fraction in the liquid phase is introduced as a primary variable, in addition to the three primary variables in the EOS3 module. A summary of EOSR3D specifications is given in Table 6.

<b>COMPONENTS</b>	#1: water #2: air #3: radionuclide
<b>PARAMETER CHOICES</b>	
(NK, NEQ, NPH, NB)=	(3,3,2,8) for isothermal condition
(NK, NEQ, NPH, NB)=	(3,4,2,8) for non-isothermal condition
<b>PRIMARY VARIABLES</b>	
single phase condition	
(P, X <sub>air</sub> , X <sub>radionuclide</sub> , T)	- (pressure, air mass fraction, radionuclide mass fraction, temperature)
two-phase condition	
(P, S <sub>g</sub> +10, X <sub>radionuclide</sub> , T)	- (pressure, gas saturation plus 10, radionuclide mass fraction, temperature)

*Table 6. Summary of EOSR3D*

### 3.9 Specification of Flow Geometry

#### Single-Phase Gas (EOS1G), Saturated/Unsaturated Flow (EOS9), and Radionuclide Transport (T2R3D) Modules

Handling of flow geometry in these modules is identical to that in TOUGH2. As in other "integral finite difference" codes (Edwards, 1972; Narasimhan and Witherspoon, 1976), flow geometry is handled by means of a list of volume elements (grid blocks) and a list of flow connections between them. This formulation can handle regular and irregular flow geometries in one, two, and three dimensions. Single- and multiple-porosity systems (porous and fractured media) can be specified, and higher order methods, such as seven- and nine-point differencing, can be implemented by means of appropriate specification of geometric data (Pruess and Bodvarsson, 1983). See Pruess et al. (1996) for further details.

### 3.10 Initial Conditions and Restarting

#### Single-Phase Gas (EOS1G), Saturated/Unsaturated Flow (EOS9), and Radionuclide Transport (T2R3D) Modules

See Section 3.10 of Pruess et al., (1996) for information pertaining to initial conditions and restarting that is also applicable to these modules. The EOS1G module has an identical procedure to that of the EOS9 module, with only one primary variable to be specified for the initial conditions. The only difference between T2R3D and EOS3 is that the mass fraction of a radionuclide is the third, and temperature is the fourth, primary variable.

### 3.11 Boundary Conditions

#### Single-Phase Gas (EOS1G), Saturated/Unsaturated Flow (EOS9), and Radionuclide Transport (T2R3D) Modules

Boundary conditions are generally specified by means of appropriately chosen volume elements, flow connections, and sinks and sources. Boundary conditions can be of two basic

types. Dirichlet conditions prescribe thermodynamic conditions, such as pressure, radionuclide concentration or temperature on the boundary, while Neumann conditions prescribe fluxes of mass or heat crossing boundary surfaces. A special case of Neumann boundary conditions is "no flux", which in the integral finite difference framework is handled by not specifying any flow conditions across the boundary. More general flux conditions are prescribed by introducing sinks or sources of appropriate strengths into the elements adjacent to the boundary. Dirichlet-type boundary conditions, such as constant pressures, concentrations and temperatures, can be specified by introducing appropriate boundary elements and connections. A connection consists of an interface area and a pair of adjacent nodes at some distance from the interface. Assigning very large volumes to such boundary elements will ensure that their thermodynamic state remains unchanged in a simulation.

### **3.12 Software and Hardware Considerations (Efficiency, Portability, etc.)**

The TOUGH2 single-phase gas flow, saturated/unsaturated flow, and radionuclide transport modules are portable to platforms that have an ANSI (FORTRAN 77) compiler. TOUGH2 can run on a PC, a Macintosh, a UNIX workstation (Sun, etc.), or a mainframe. They are easily maintained because of the flexibility of their modularization and through their internal version control, which allows the user to note version updates and to document personalized changes to the program.

The TOUGH2 ECM Module is also portable to platforms that have an ANSI (FORTRAN 77) compiler. It can also run on a PC, a Macintosh, a UNIX workstation (Sun, etc.), or a mainframe.

### **3.13 Performance Requirements and Design Constraints**

#### Single-Phase Gas (EOS1G) and Saturated/Unsaturated Flow (EOS9)

See Section 3.13 of Pruess et al. (1996) for a description of performance requirements and design constraints that are also applicable to these modules.

#### Radionuclide Transport Module (T2R3D)

The discussion of Pruess et al. (1996) for performance requirements and design constraints are, in principle, applicable to the T2R3D model. However, application of the T2R3D program to a field problem is subject to several additional limitations due to the model assumptions and the numerical schemes implemented. It is critical for the user to recognize those limitations before applying the code. First, the radionuclide is treated as a liquid tracer, and has no effects on fluid properties. This implies that T2R3D cannot be used for strongly coupled flow and transport problems in which fluid properties are significantly affected by the solute concentrations. Second, effects of heat on transport properties, such as  $K_r$ , or diffusion coefficients, of a radionuclide are ignored because of the lack of the related research in these areas, even though T2R3D has the capability to model a fully-coupled hydrologic-thermal-chemical (H-T-C) problem. Like the TOUGH2 code, T2R3D can be easily modified to include thermal effects on radionuclide transport once the constitutive correlations of these couplings are known. Also we benchmark the numerical simulation results against analytical solutions only under isothermal and saturated cases in this report. For a general non-isothermal transport problem with phase changes no analytical solutions are available, and the model verification will be difficult to conduct currently. Third, the averaging schemes of T2R3D for the velocity and the concentration gradient vectors are based on

our physical analysis and a limited number of numerical tests in which the numerical simulations match analytical solutions. A further study is certainly needed since a universally applicable averaging scheme may not exist for a general irregular grid in a heterogeneous system. Last, caution must be taken in selecting spatial and time discretizations, and the user should check the Peclet number and the Courant number in analyzing the simulation results. T2R3D, like TOUGH2, is designed with consideration of accuracy, efficiency, general purpose, flexibility and robustness, and these objectives may conflict with each other for certain applications. In many cases, it is the choice the user has to make. For example, the ECM method is not recommended to use with the T2R3D simulation unless a steady-state solution is sought for radionuclide transport in fractured porous media.

### 3.14 Future Developments

Development of the single-phase Gas Module of TOUGH2 (EOS1G), and the Saturated/Unsaturated Flow Module (EOS9) are complete. Future development of the Radionuclide Transport Module (T2R3D) may be focused on work to:

- (1) include a multi-member radionuclide decay chain;
- (2) consider possible radionuclide transport mechanism in the gas phase; and
- (3) decouple flow and transport simulations to improve computational efficiency for large 3-D problems.

There are no plans for further development of the Effective Continuum Method Formulation Module (ECM), at this time.

### 3.15 Verification of Design Description

#### Single-Phase Gas Flow Module (EOS1G)

Verification that the TOUGH2 single-phase Gas Module meets the design description and structure depicted in Figure 3 was conducted during testing and debugging of the code. Sample runs were set up to test the ability of the EOS modules to handle primary variables in the manner described above. Once the runs were completed, sample problems were constructed to demonstrate the code. These are found in Appendix C.

#### Effective Continuum Method Formulation Module (ECM)

Verification that the TOUGH2 ECM Formulation Module meets the design description and structure depicted in Figure 3 was conducted during testing and debugging of the code. Sample runs were set up to test the ability of the ECM module to handle relative permeability and capillary pressure functions as described by the formulation. Once the runs were completed, sample problems were constructed to demonstrate the code. These are found in Appendix C.

#### Saturated/Unsaturated Flow Module (EOS9)

Verification that the TOUGH2 Saturated/Unsaturated Flow Module meets the design description and structure depicted in Figure 3 was conducted during testing and debugging of the code. Sample runs were set up to test the ability of the EOS modules to handle primary variables in the manner described above. Once the runs were completed, sample problems were constructed to demonstrate the code. These are found in Appendix C.

### Radionuclide Transport Module (T2R3D)

Verification that T2R3D meets the design description was conducted during testing and debugging of the code. The code has been applied to a number of radionuclide transport simulation problems at Yucca Mountain, and a sample problem was constructed and included in Appendix C.



## 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 in Section 2.1. The terms “verification” and “validation” are used differently in quality assurance software than in scientific research. In quality assurance terms, “software verification” means checking to ensure that a following stage (e.g. implementation) fulfills the requirements of a preceding stage (e.g. design), where the Software Life Cycle is built on a “waterfall approach” in which requirements are established, followed by code design, then code implementation, and finally validation. Validation means that the operational code satisfies all the requirements specified for it in the requirements stage.

#### 4.1.1 Acceptance Criteria

##### Single-Phase Gas (EOS1G), Saturated/Unsaturated Flow (EOS9), and Radionuclide Transport (T2R3D) Modules

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

The acceptance criteria for these TOUGH2 modules are the same as those used for standard TOUGH2 (Pruess et al., 1996). The acceptance criterion for establishing that each module's results showed sufficient agreement to the analytical solution was demonstration that the obtained results for TOUGH2 and the analytical solution differed by five percent or less (95% or better agreement). The five percent error is defined as a relative error, i.e., the difference between TOUGH2 and analytical solutions relative to the maximum changes in the time and spatial domain for the concerned primary variables, such as pressure, saturation, mass fraction and temperature. The five percent choice is somewhat arbitrary; depending upon the nature of the problem, it may be possible (and is always desirable) to achieve much closer agreement. The validation problems are summarized in Table 7. A short summary of each, along with a graphical comparison of each module and the analytical solution, is found in the following paragraphs. For some applications, comparison could not be made to an analytical solution but could be made to experimental results in the field. In the context of scientific conceptual models, this type of comparison is called “model validation”. Comparisons of TOUGH2 module solutions with experimental results are also included in Table 7 and are described in the following section along with a graphical comparison. Acceptance criteria are difficult to quantify for comparisons against experimental or field data because the closeness of fit will depend partly on the goodness of original data, experimental artifacts, and heterogeneity in the natural system. Where possible, we try to obtain an agreement of 90% or better. A 95% or better agreement with analytical solutions, or a 90% or better agreement with laboratory or field data will sufficiently ensure the correctness of the formulation and description of the physical processes of the code.

In the terminology of software engineering, “validation” tests are those that ensure that the software meets the requirements specified for it. The “verification” tests also fulfill the definition of “software validation”, because in order to obtain good results when compared to analytical solutions, the software must be able to model the processes of interest in the problem.

## Effective Continuum Method Formulation Module (ECM)

The ECM formulation is a theory, dependant on the local thermodynamic equilibrium assumptions. The ECM module will give reasonable results for fracture-matrix flow as long as the underlying assumption is valid.

#	Problem Title	Dimensions	Features	Issues	References
1	Single-phase gas flow (EOS1G)	1-D, linear vertical	non-isothermal two-phase	code verification against TOUGH2 EOS3 module	this paper
2	Comparison of ECM and dual-permeability models (EOS3)	1-D, linear, vertical	isothermal, two-phase, heterogeneous, fracture and matrix flow	demonstration of applicability of ECM	this paper
3	Infiltration (EOS3)	1-D, linear, vertical	isothermal, two-phase	verification of the code against semi-analytical and numerical solutions	this paper and Pruess et al., (1996)
4	1-D transport with dispersion and diffusion (EOSR3D)	1-D, linear, horizontal	isothermal, dispersive flux in liquid	verification of the code against an analytical solution	this paper
5	2-D transport with dispersion and diffusion (EOSR3D)	2-D, horizontal	isothermal, longitudinal and transverse dispersive flux in liquid	verification of the code against an analytical solution	this paper

*Table 7. Summary of Validation Problems for TOUGH2 Modules*

### 4.2 Validation Tests (Keyed to Table 7)

#### Single-Phase Gas Flow Module (EOS1G)

##### 1. Single-Phase Transient Gas Flow (this paper)

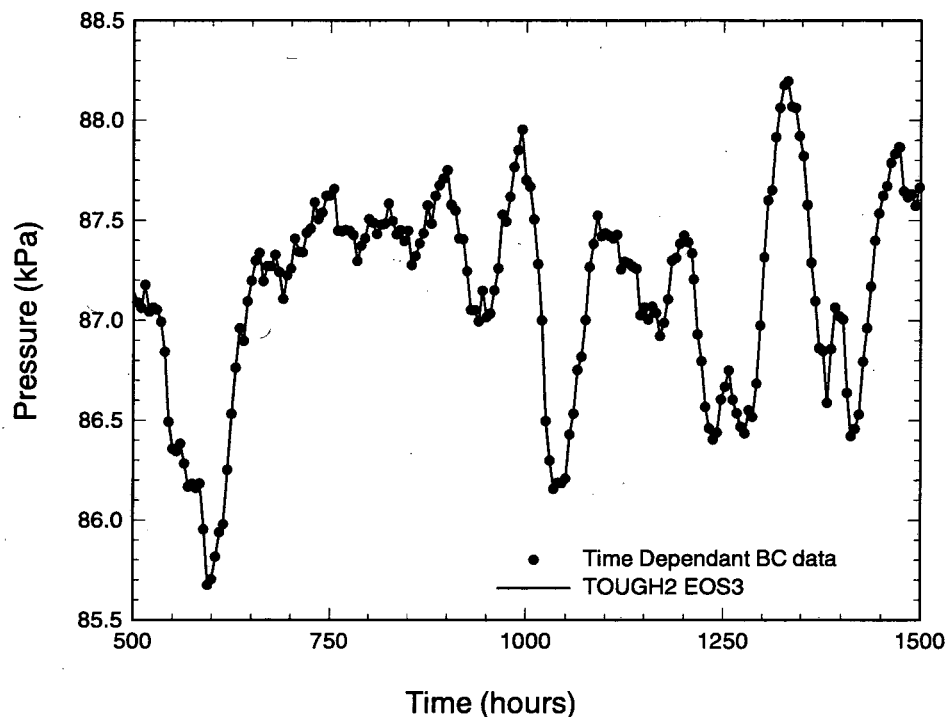
In this problem we compare the results of a transient gas flow simulation using the single-phase gas module (EOS1G) with results using the previously validated EOS3 module. This problem is also used to validate a new treatment in TOUGH2 for time-dependent pressure boundary conditions.

A one dimensional grid of 99 grid blocks is arranged vertically with one meter spacing between grid blocks. Steady-state initial conditions are gas static pressures with the bottom pressure at 90 kPa, a uniform temperature gradient from 30 °C at the lower boundary to 10 °C at the upper boundary, and variable liquid saturation from 0.99 at the lower boundary to 0.57 at the upper boundary. Air solubility in liquid water is represented by Henry's law, as treated in the

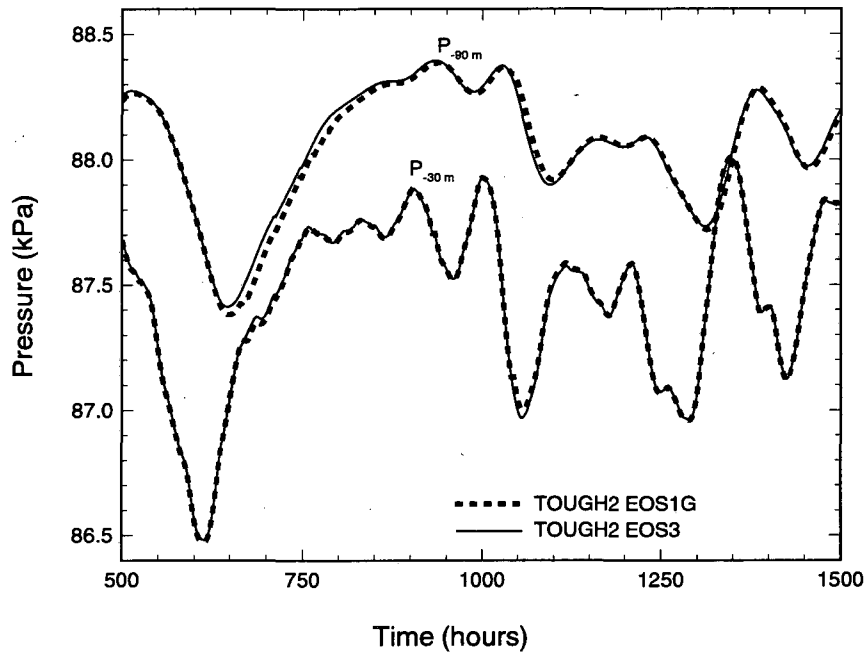
EOS3 module (Pruess et al., 1996). Variable liquid saturation is initialized by running the TOUGH2 EOS3 and assuming 1 mm/year water infiltration into the upper boundary, capillary suction characteristic of Yucca Mountain tuffs (van Genuchten model with  $\alpha = 0.0000167 \text{ Pa}^{-1}$  and  $m = 0.167$ ), and a Brooks-Corey relative permeability function. These parameters are unchanged for the comparison simulations, except that no liquid source term was used with the single-phase gas module. Other relevant parameters are 100 microdarcys absolute permeability and 0.01 porosity. The upper pressure boundary condition is time varying and is provided by tabular input to TOUGH2. All other boundaries are no-flow. A constant time step of two hours is used in the simulations.

A comparison of the TOUGH2 simulated time-varying pressures at the upper boundary and the time and pressure data provided to TOUGH2 is shown in Figure 8. Figure 8 indicates that there is nearly perfect agreement between the simulation and the data, much better than the required 95%.

A comparison of pressure response at 30 m and 90 m below the upper boundary simulated using the single-phase gas module (EOS1G) and EOS3 is shown in Figure 9. Figure 9 indicates that the agreement between the results using the validated EOS3 module and the new single-phase gas module (EOS1G) is very good at 30 m and also at 90 m near the bottom boundary of the model. Actually, the results show that the agreement between the two modules is excellent for each gridblock at each time step. Therefore, the acceptance criteria for EOS1G are satisfied.



**Figure 8.** Time dependent pressures for the boundary condition data input table to TOUGH2 and the TOUGH2 simulated boundary pressures

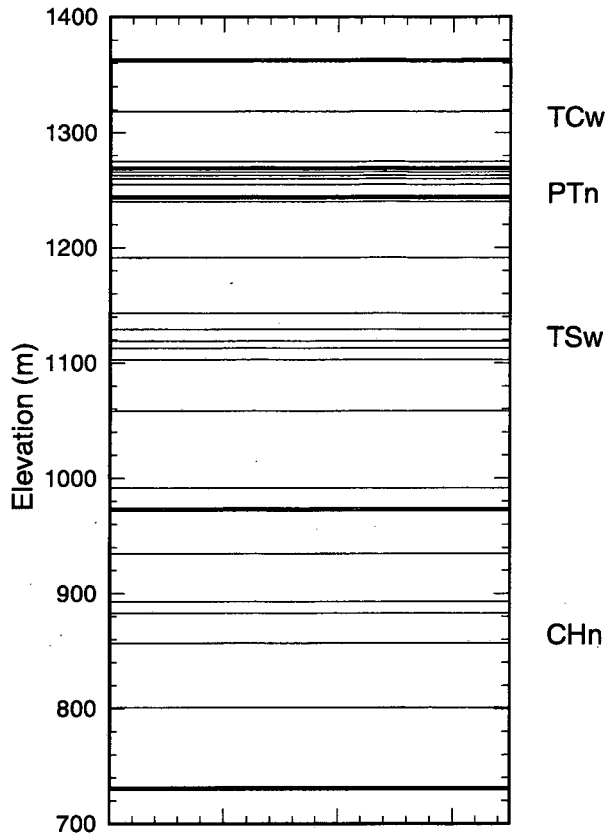


**Figure 9.** Time dependent pressures for the TOUGH2 simulations using the EOS3 module and the single-phase gas module (EOS1G)

### Effective Continuum Method Formulation Module (ECM)

#### 2. A comparison of the ECM and dual-permeability modeling approaches (this paper)

This is a one-dimensional vertical flow problem in an unsaturated zone of Yucca Mountain and a single vertical column grid is extracted directly from the 3-D site-scale model (Bodvarsson and Bandurraga, eds., 1996), as shown in Figure 10. It consists of 24 active grid blocks, 3 for the Tiva Canyon unit (TCw), 5 for the Paintbrush (PTn), 10 for the Topopah Springs (TSw), and 6 for the Calico Hills (CHn), and an overlying and underlying boundary block representing the atmosphere and the water table conditions, respectively. The fracture system in the unsaturated zone of the mountain is also subdivided into the same four units, TCw, PTn, TSw, and CHn. The properties of fractures are taken from TSPA-93 (Wilson et al., 1994) for the four units, as listed in Table 8.



**Figure 10.** One-dimensional vertical grid for the unsaturated zone of Yucca Mountain, used for the ECM comparison study.

Unit	Porosity	Spacing (m)
TCw	1.38e-3	0.618
PTn	4.12e-3	2.220
TSw	2.75e-3	0.740
CHn	9.98e-4	1.618

**Table 8.** The fracture porosity and spacing data used for the comparison study (Wilson et al., 1994).

Since few fractures exist in the PTn unit, the effects of fractures on moisture flow in the PTn are ignored in this simulation, and the PTn formation is treated as a single porous medium rock. The same set of matrix and fracture properties, as listed in Table 9, are used for both ECM and dual-permeability simulations.

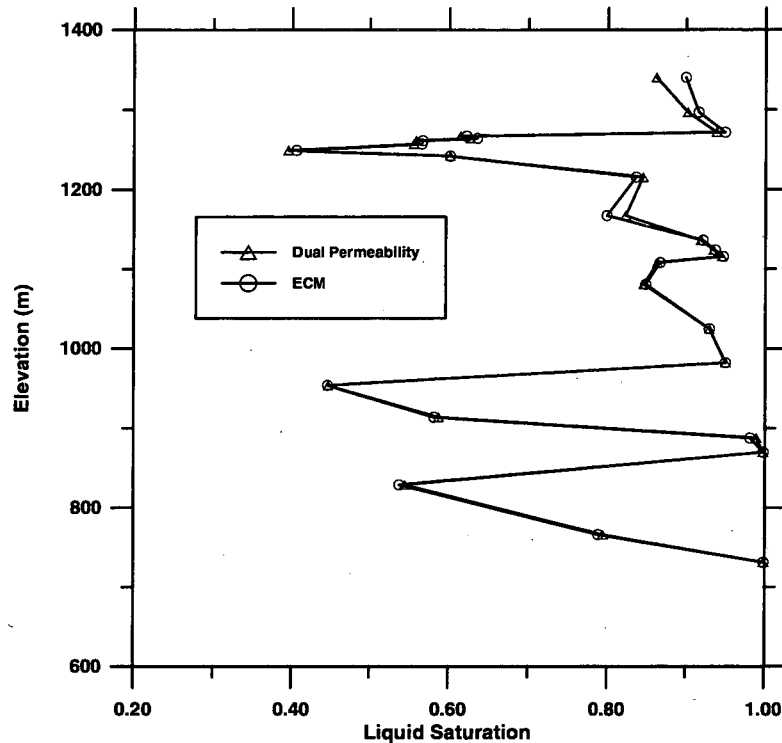
Units	$k_m$ (m <sup>2</sup> )	$k_f$ (m <sup>2</sup> )	$\alpha_m$ (Pa <sup>-1</sup> )	$\alpha_f$ (Pa <sup>-1</sup> )	$m_m$	$m_f$	$\phi_m$	$\phi_f$
tcw11	0.160E-18	0.910E-11	0.147E-04	0.518E-03	0.238	0.182	0.062	0.290E-03
tcw12	0.540E-15	0.575E-11	0.174E-05	0.977E-03	0.233	0.223	0.082	0.290E-03
tcw13	0.220E-16	0.575E-11	0.129E-05	0.123E-02	0.463	0.437	0.207	0.290E-03
ptn21	0.400E-12	n/a	0.244E-04	n/a	0.215	n/a	0.435	n/a
ptn22	0.240E-12	n/a	0.159E-04	n/a	0.310	n/a	0.222	n/a
ptn23	0.111E-12	n/a	0.445E-04	n/a	0.243	n/a	0.406	n/a
ptn24	0.880E-13	n/a	0.341E-04	n/a	0.295	n/a	0.499	n/a
ptn25	0.105E-11	n/a	0.138E-03	n/a	0.243	n/a	0.490	n/a
tsw31	0.261E-12	0.400E-11	0.237E-04	0.122E-02	0.206	0.203	0.048	0.243E-03
tsw32	0.194E-12	0.445E-11	0.172E-04	0.969E-03	0.248	0.249	0.156	0.243E-03
tsw33	0.796E-17	0.743E-11	0.573E-05	0.243E-03	0.247	0.250	0.154	0.243E-03
tsw34	0.100E-14	0.159E-11	0.754E-06	0.686E-03	0.321	0.325	0.110	0.243E-03
tsw35	0.423E-15	0.400E-11	0.234E-05	0.108E-02	0.231	0.226	0.130	0.243E-03
tsw36	0.776E-16	0.400E-11	0.522E-06	0.122E-02	0.416	0.416	0.112	0.243E-03
tsw37	0.316E-15	0.400E-11	0.804E-06	0.122E-02	0.368	0.368	0.036	0.243E-03
ch1vc	0.160E-11	0.723E-12	0.760E-04	0.122E-02	0.221	0.227	0.273	0.111E-03
ch2vc	0.550E-13	0.723E-12	0.980E-04	0.122E-02	0.223	0.227	0.344	0.111E-03
ch3zc	0.450E-17	0.100E-12	0.394E-05	0.388E-03	0.225	0.225	0.332	0.525E-04
ch4zc	0.210E-16	0.100E-12	0.150E-06	0.730E-03	0.475	0.470	0.266	0.525E-04
pp3vp	0.542E-14	0.300E-13	0.194E-04	0.122E-02	0.316	0.313	0.322	0.111E-03
pp2zp	0.269E-15	0.100E-12	0.126E-05	0.730E-03	0.311	0.312	0.286	0.525E-04

*Table 9. The rock properties of matrix and fractures used in the ECM comparison study.*

In this table,  $k_m$  and  $k_f$  are saturated matrix and fracture continuum permeabilities;  $\alpha_m$  and  $\alpha_f$  are van Genuchten's parameter of capillary pressure of matrix and fracture;  $m_m$  and  $m_f$  are van Genuchten's parameter of soil retention curves; and  $\phi_m$  and  $\phi_f$  are porosities of matrix and fracture systems, respectively.

The same boundary conditions are specified for both models as Dirichlet-type conditions, i.e., constant pressures, temperatures and saturation. Also the surface boundary is subject to a constant water infiltration of 3.6 mm/year. However, the water infiltration on the ground surface is only added into the fracture elements on the top boundary for the dual-permeability model, while it is distributed between fracture and matrix in the ECM model because, realistically, infiltration is expected almost entirely through the fractures, but the continuum approach of the ECM uses equilibrium partitioning for the infiltration. Also an isothermal condition was assumed to exist under two-phase flow conditions.

Both models are run to steady-state, and the simulation results are shown in Figure 11.



*Figure 11. Steady-state liquid saturation profiles for fractures and matrix, obtained using the ECM and the dual-permeability models.*

Figure 11 shows the steady-state liquid saturation profiles for fractures and matrix, obtained using the ECM and the dual-permeability models. Figure 11 shows that almost identical results of matrix saturations are obtained from the two modeling approaches. The only differences between the two solutions may be noticed in the TCw unit, or along the interfaces between the PTn and the TSw. The reasons for these minor differences are from the conceptual model, rather than from the modeling approaches. First, the water infiltration is imposed into fractures only on the top boundary in the dual-permeability simulation, while the ECM model puts the infiltration into both fracture and matrix systems. Second, the PTn unit is treated as a single porous medium, and this creates certain discontinuities in matrix/fracture vertical connections across the interfaces.

Figure 11 indicates that as long as the local equilibrium condition is satisfied between the fracture and matrix systems, the ECM formulation will give accurate predictions of saturation distributions. We can create a situation under which the local equilibrium condition is not well satisfied, and the ECM approach will introduce considerable errors into the solution. Figure 12 shows a comparison for simulated liquid saturation profiles also using the ECM and the dual-permeability methods. However, the interface areas between the fracture and matrix systems were reduced by a factor of 10, 100, and 1,000, respectively. The interface areas become 10%, 1%, and 0.1% of the geometric area of the fracture and matrix systems, as shown in Figure 12. As the fracture-matrix interface areas get smaller, the local equilibrium conditions are less well satisfied, and the figure shows more differences between the predictions using the ECM and the dual-permeability approaches for the top, the TCw unit, and the middle, TSw, unit. Figure 12 also shows that even with many orders of magnitude reduction in the fracture-matrix interface areas, the comparisons are still good between the ECM and the dual-permeability methods for the lower unit of CHn. The reason is that the fractures are less permeable in that unit, relative to the permeability of the matrix, and the local equilibrium conditions are still reasonable.

This problem shows that the ECM formulation will give an accurate description of matrix/fracture flow at steady-state flow conditions or as long as the model assumptions are closely satisfied.

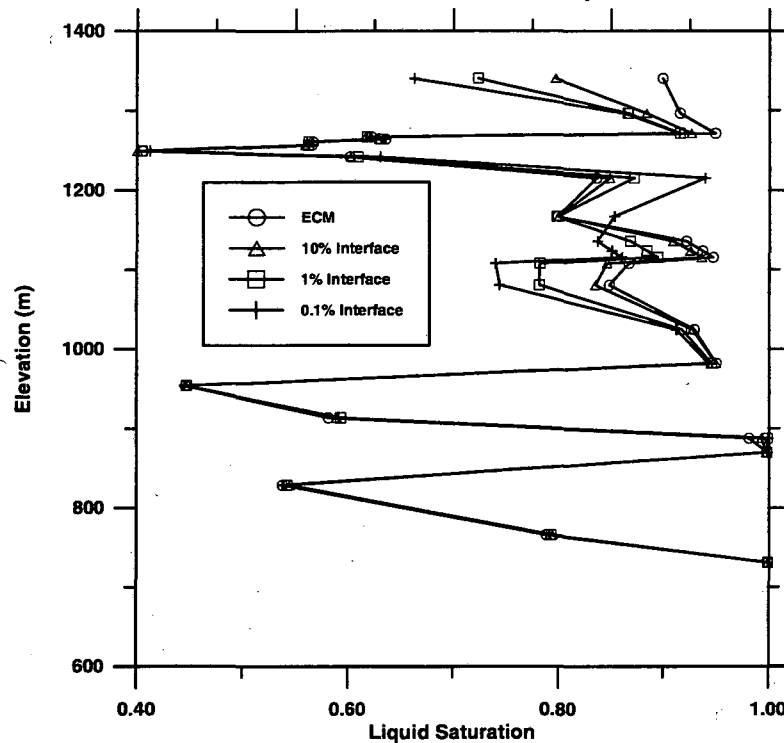


Figure 12. Comparison of the simulated liquid saturation profiles using the ECM and the dual-permeability models with reduction of fracture-matrix interface areas.

### Saturated/Unsaturated Flow Module (EOS9)

#### 3. 1-D Linear Infiltration (Pruess, 1987; Ross et al., 1982; Philip, 1955)

This is a one-dimensional problem that considers infiltration into a semi-infinite tube of partially saturated soil. Philip (1955) obtained a semi-analytical solution for this problem, using a similarity transformation method. Detailed specifications were given in a report by Ross et al. (1982), who proposed this problem as a benchmark case for numerical simulators. The infiltration boundary in the problem is represented by means of a very large element, with a nodal distance set to a small non-zero value, to avoid relative permeability at the boundary being taken from the underlying element. Both the solution obtained by Philip (1955) and EOS9 treat the gas phase as a passive phase at constant pressure. In contrast, for EOS3 this approximation must be enforced by surrounding the soil tube with a ring of very large volume, which is assigned a pressure of  $P = 1$  bar. Figure 13 shows that the EOS3 and EOS9 solutions match each other very closely, and agree well with the semi-analytical solution given by Ross et al. (1982), meeting the acceptance criterion of 95% or better agreement. For this problem EOS9 runs about three times faster than EOS3.



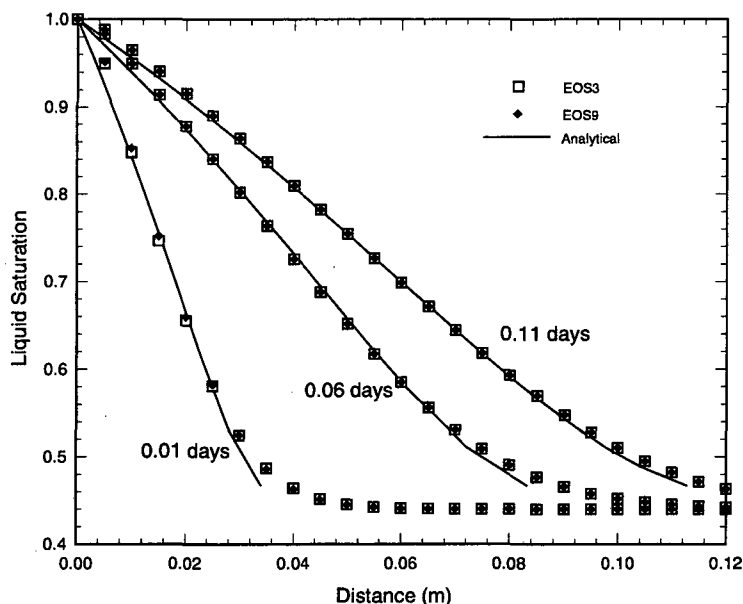


Figure 13. Liquid saturation profiles for TOUGH2 verification problem 1, using EOS9 and EOS3 and harmonic-mean interface weighting of mobilities

#### Radionuclide Transport Module (T2R3D)

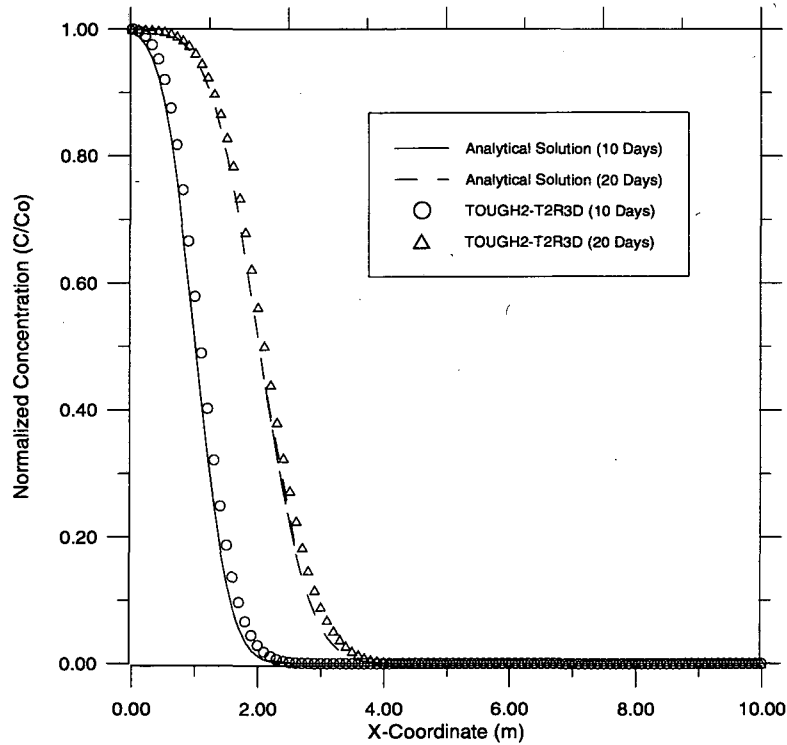
#### 4. One-Dimensional Transport with dispersion and diffusion (this paper)

This problem is designed to examine the accuracy of the T2R3D code in simulating radionuclide or tracer transport in the liquid phase with hydraulic dispersion and molecular diffusion and is similar to the one used by Oldenburg and Pruess (1993) to verify a two-dimensional transport module of TOUGH2. The problem concerns one-dimensional transport of a radionuclide in a homogeneous saturated porous medium 10 meters long. The flow field is steady-state with 0.1 m/day velocity. A radionuclide is introduced at the inlet ( $x=0$ ) with a constant concentration, and transport starts at  $t=0$  by advection, hydraulic dispersion, and diffusion. An analytical solution for this problem is provided by Javandel et al. (1984), and it is used here to verify the T2R3D numerical solution.

The T2R3D solution of this problem is accomplished by specifying both inlet and outlet boundary elements with constant pressures, which give rise to a steady state flow field of 0.1 m/day pore velocity. In the T2R3D simulation, a one-dimensional, uniform linear grid of 1,000 elements was generated using the TOUGH2 MESHMAKER for the 10-meter domain. In order to eliminate effects of two-phase and non-isothermal flow, air mass fraction is set to zero and a constant temperature of 25 °C is specified. Also no decay or adsorption effects are included. The properties used in the comparison are: porosity  $\phi = 1$ ; tortuosity  $\tau = 1$ , molecular diffusion coefficient  $D_m = 1.0 \times 10^{-10}$  m<sup>2</sup>/s, longitudinal dispersivity  $\alpha_L$  is 0.1 m. The liquid properties are internally generated by the code. Initially there is no radionuclide in the system;  $X^{\text{radionuclide}} = 1.0 \times 10^{-5}$  at the inlet boundary ( $x = 0$ ); and  $X^{\text{radionuclide}} = 0$  at the outlet boundary at all times.

A comparison of the normalized radionuclide concentrations along the rock column from the T2R3D and analytical solution is shown in Figure 14 for  $t=10$  and 20 days, respectively. The

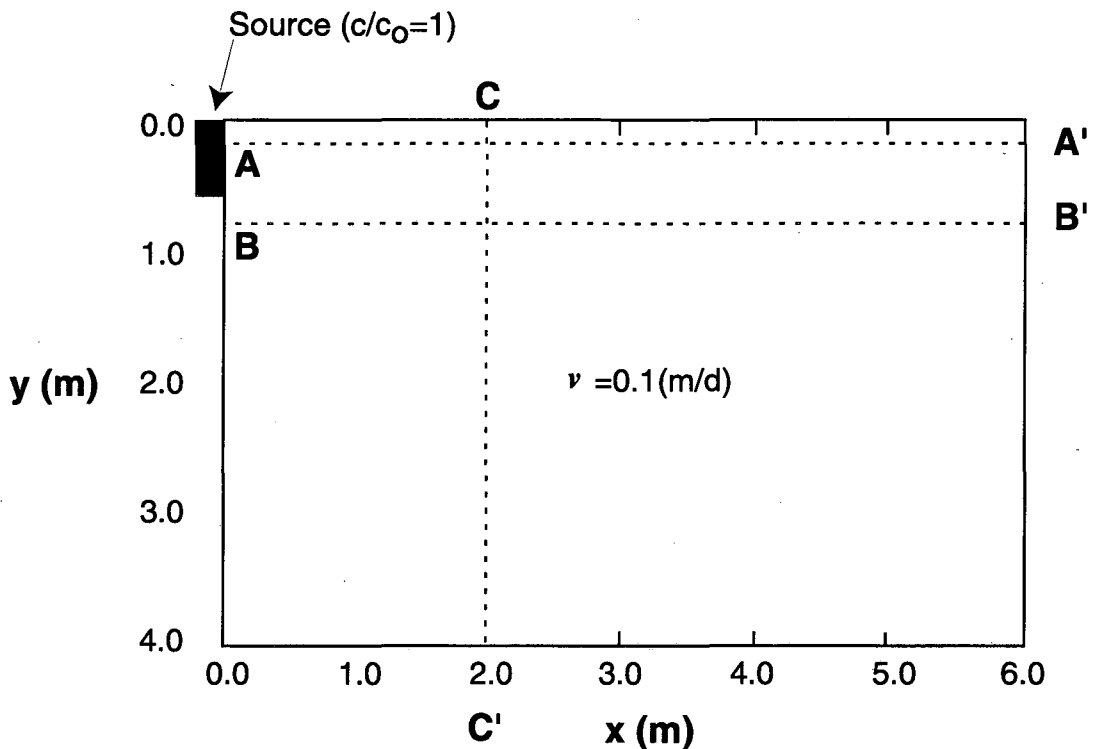
figure indicates that the T2R3D simulated concentration profiles are in excellent agreement with the analytical solution, and meet the acceptance criteria of having 5% or less discrepancy from the analytical solution.



*Figure 14. Comparison of the normalized radionuclide concentrations along the rock column from the T2R3D and analytical solution*

## 5. Two-Dimensional Transport with dispersion and diffusion (this paper)

This problem is designed to examine the accuracy of the T2R3D code in handling radionuclide transport in a multi-dimensional domain with hydraulic dispersion and molecular diffusion effects. The problem is similar to the one used by Oldenburg and Pruess (1993). The problem concerns two-dimensional transport of a radionuclide in a homogenous isotropic, saturated porous medium. The model domain is rectangular, as shown in Figure 15. There is a steady-state, one-dimensional flow field along the x-direction with pore velocity of 0.1 m/day within the domain. A radionuclide is introduced along a line source of length of 0.5 meter at  $x=0$  with a constant concentration. Transport starts at  $t=0$  from the line source by advection, hydraulic dispersion and diffusion. An analytical solution for this problem is provided by Javandel et al. (1984) along with a code for calculating the 2-D concentrations. The analytical solution is used here to verify the T2R3D numerical solution.

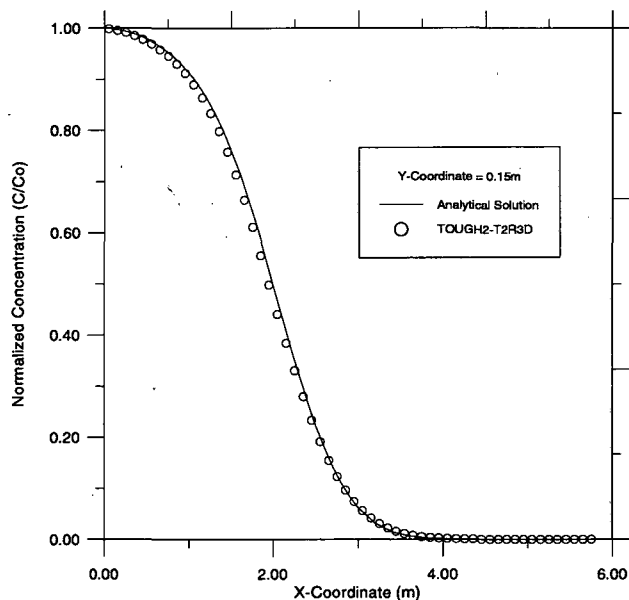


**Figure 15.** Schematic of the 2-D model domain for the two-dimensional radionuclide transport problem showing the velocity field and three cross sections for comparisons of the simulation results.

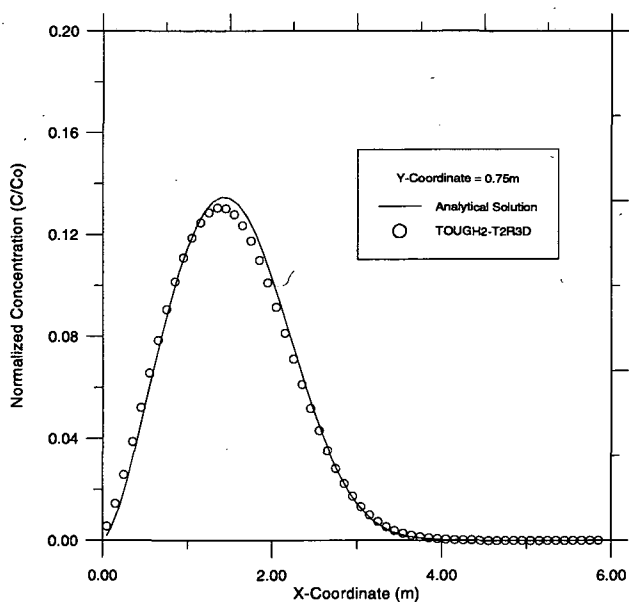
The T2R3D solution of this problem is accomplished by specifying on both the upstream boundary ( $x=0$ ) and downstream boundary ( $x=6$  m) a constant pressure, which gives rise to a steady-state flow field of 0.1 m/day flow velocity. Also, in the T2R3D simulation, a uniform grid spacing was used for both  $x$  and  $y$  directions with  $\Delta x = \Delta y = 0.1$  m. The grid was generated using the TOUGH2 MESHMAKER. As in the one-dimensional transport case discussed above, the system is kept at single liquid-phase and isothermal conditions. Air mass fraction is set to zero and a constant temperature of 25 °C is specified. Also no decay or adsorption effects are included in the simulation. The properties used in the comparison study are: porosity  $\phi = 1$ , tortuosity  $\tau = 1$ , molecular diffusion coefficient  $D_m = 1.0 \times 10^{-10}$  m<sup>2</sup>/s, longitudinal dispersivity  $\alpha_L$  is 0.1 m, and transverse dispersivity  $\alpha_T$  is 0.025 m. The liquid properties are internally generated by the code. The initial and boundary conditions for the radionuclide are: initially there is no radionuclide in the system;  $X^{\text{radionuclide}} = 1.0 \times 10^{-5}$  along the 0.5 m line source; and  $X^{\text{radionuclide}} = 0$  at the downstream boundary ( $x=6$  m) at all times.

Comparison of the normalized radionuclide concentrations along the three cross-sections of the rock column from the T2R3D and the analytical solution are shown in Figures 16, 17, and 18 for  $t = 20$  days, respectively. The figures indicate that the T2R3D simulated concentration profiles in the two-dimensional domain are in good agreement with the analytical solution. Figure 16 shows the radionuclide profile at  $y=0.15$  m (cross section A-A' in Figure 15), indicating an excellent agreement between the two solutions along this cross section. Figure 17 shows the concentration profile at  $y = 0.75$  m, just below the line source which extends from  $y = 0$  to  $y = 0.5$  m, and this figure displays both longitudinal and transverse dispersion effects. As can be seen in Figure 17, the comparison is good even though small numerical errors are introduced in

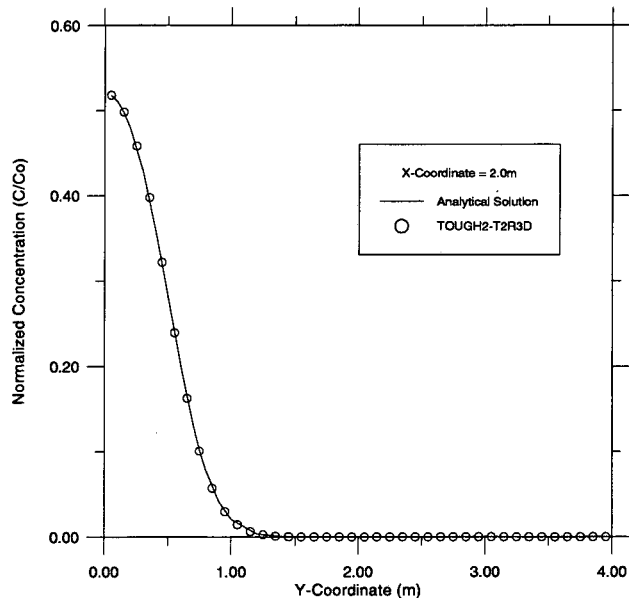
the numerical solution. Figure 18 gives the comparison of concentration profiles along the transverse direction (C-C') at  $x = 2$  m, indicating an excellent agreement between the analytical and numerical solutions at this location. The examination of the simulation results of Figure 16 to 18 indicates that they meet the acceptance criteria of having 5% or less discrepancy from the analytical solution.



*Figure 16. Comparison of radionuclide concentration profiles at along cross section (A-A') for analytical and numerical solutions at  $t=20$  days*



*Figure 17. Comparison of radionuclide concentration profiles at along cross section (B-B') for analytical and numerical solutions at  $t=20$  days.*



*Figure 18. Comparison of radionuclide concentration profiles at along cross section (C-C') for analytical and numerical solutions at t=20 days.*

### 4.3 Summary

#### Single-Phase Gas Flow Module (EOS1G)

Verification of the TOUGH2 EOS1G module was accomplished by using the previously-validated TOUGH2 EOS3 module for a transient gas flow problem. The two modules provided virtually identical simulation results for gas flow.

#### Effective Continuum Method Formulation Module (ECM)

The ECM model assumptions and applicability to a Yucca Mountain field problem were demonstrated in this section. The comparison of results from the ECM and the dual-permeability formulations indicates that at steady-state or as long as the local thermodynamic conditions are approximately satisfied in a fractured porous medium, the ECM formation will provide a very accurate description of the fracture/matrix flow system, in terms of moisture flow and distribution.

#### Saturated/Unsaturated Flow Module (EOS9)

Verification of the TOUGH2 EOS9 module was accomplished by using both the previously-validated TOUGH2 EOS3 module and a semi-analytical solution for a transient infiltration problem of variably saturated soil. The two EOS modules and the analytical solution were all in excellent agreement.

### Radionuclide Transport Module (T2R3D)

Verification of the T2R3D module was accomplished by using two verification examples, which compared the T2R3D simulations results with the analytical solution in one- and two-dimensional systems of radionuclide transport. In both cases, the T2R3D numerical solutions were in good agreement with the analytical solutions.

As a demonstration that specified requirements have been met for the four TOUGH2 modules (Single-Phase Gas Flow, Effective Continuum Method, Saturated/Unsaturated Flow and Radionuclide Transport), Table 10 provides a cross-check of the requirements against the validation problems described above that satisfy those requirements.

Requirement	Test Case	Criteria Met?	Reference
<b>Single-Phase Gas (EOS1G) and Saturated/Unsaturated Flow (EOS9) Modules</b>			
A. Flow processes driven by pressure, viscous, capillary, and gravity forces			
- single-phase gas flow in two-phase existing conditions (EOS1G)	1	met	this paper
- single-phase water flow in two-phase or single-liquid phase conditions (EOS9)	3	met	this paper
B. Physics			
- accurate description of thermophysical properties of water, vapor, and air	1, 3	met	this paper
- dissolution of air in water	1	met	this paper
C. Phase change and interaction			
- interference between liquid and gas phases		met	Pruess et al., 1996
D. Stable, but non-uniform temperature distribution	1	met	this paper
E. Dimensionality			
- 1-D, 2-D, and 3-D flows		met	Pruess et al., 1996
F. Geometry			
- Cartesian, cylindrical, irregular	8, 9, 16	met	Pruess et al., 1996
G. Grid generation	8, 12	met	Pruess et al., 1996
H. Heterogeneities			
- heterogeneous formations	8, 18	met	Pruess et al., 1996
- flow in porous and fractured media	7, 8, 11	met	Pruess et al., 1996
I. Flexible specification of initial and boundary conditions, sources and sinks	1, 3	met	this paper
J. Other			
- automatic time-stepping	all cases	met	Pruess et al., 1996
- restart capability	NA	met	Pruess et al., 1996
- sample problems to illustrate code use, verify accuracy	1, 3	met	this paper
- internal version control	1, 3	met	this paper
<b>Effective Continuum Method Formulation (ECM) Module</b>			
A. Constitutive correlations: accurate description of relative permeability and capillary pressure functions under local thermodynamic equilibrium assumption.	2	met	this paper
<b>Radionuclide Transport (T2R3D) Module</b>			
A. Flow processes driven by pressure, viscous, capillary, and gravity forces	4, 5	met	this paper
- two-phase flow of liquid and gas (air and vapor)	3, 8, 10	met	Pruess et al., 1996
B. Physics			
- accurate description of thermophysical properties of water, vapor, and air	13	met	Pruess et al., 1996
- binary diffusion of air and water components in gas phase	3, 17b	met	Pruess et al., 1996
- binary diffusion and hydrodynamic dispersion of radionuclides in liquid phase	4, 5	met	this paper

Table 10. Requirements Validation Cross-Check

Requirement	Test Case	Criteria Met?	Reference
<b>C. Phase change and interaction</b>			
- appearance and disappearance of phases	7, 10	met	Pruess et al., 1996
- interference between liquid and gas phases	3, 8, 10	met	Pruess et al., 1996
- enhancement of gas phase permeability from Knudsen (slip flow) effects	17c	met	Pruess et al., 1996
- vapor-liquid phase change	2, 3, 10	met	Pruess et al., 1996
<b>D. Heat transport</b>			
- heat conduction	7, 12	met	Pruess et al., 1996
- heat convection	4, 5, 9	met	Pruess et al., 1996
- sensible and latent heat changes	2, 3, 5	met	Pruess et al., 1996
- conductive heat exchange with impermeable strata	7, 12	met	Pruess et al., 1996
- coupled fluid and heat flow	2, 3, 4	met	Pruess et al., 1996
<b>E. Dimensionality</b>			
- 1-D, 2-D, and 3-D flows	1, 8, 18	met	Pruess et al., 1996
<b>F. Geometry</b>			
- Cartesian, cylindrical, irregular	8, 9, 16	met	Pruess et al., 1996
<b>G. Grid generation</b>			
	8, 12	met	Pruess et al., 1996
<b>H. Heterogeneities</b>			
- heterogeneous formations	8, 18	met	Pruess et al., 1996
- flow in porous and fractured media	7, 8, 11	met	Pruess et al., 1996
<b>I. Flexible specification of initial and boundary conditions, sources and sinks</b>			
	4, 5	met	this paper
<b>J. Other</b>			
- automatic time-stepping	all cases	met	Pruess et al., 1996
- restart capability	NA	met	Pruess et al., 1996
- sample problems to illustrate code use and verify accuracy	4, 5	met	this paper
- internal version control	4, 5	met	this paper
- modularized structure for modifying or adding capabilities	4, 5	met	this paper

*Table 10, cont. Requirements Validation Cross-Check.*



## 5. SOFTWARE USER DOCUMENTATION

### 5.1 Installation Procedures

#### Single-Phase Gas (EOS1G), Effective Continuum Method (ECM), Saturated/Unsaturated Flow (EOS9) and Radionuclide Transport (T2R3D) Modules

The distribution media for TOUGH2 and its modules vary. For installation options on a work station or mainframe, information should be obtained from the ESTSC distribution center at Oak Ridge. For a PC, the program is installed by inserting the diskette into the appropriate disk drive and typing "install". Instructions for operating TOUGH2 will appear in the TOUGH2 "README" file, which is included as Appendix D to this document.

### 5.2 Hardware and Software Operating Environments

#### Single-Phase Gas (EOS1G), Effective Continuum Method (ECM), Saturated/Unsaturated Flow (EOS9) and Radionuclide Transport (T2R3D) Modules

As stated previously, TOUGH2 and its modules can be operated in any type of environment: on a mainframe computer, at a workstation, and on a PC or a Macintosh.

### 5.3 Input and Output

#### 5.3.1 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), with the exception that only a single parameter is specified. For code nomenclature see Appendix E.

#### 5.3.2 Effective Continuum Method Formulation Module (ECM)

The following equations define the input parameters for the ECM module.

The van Genuchten function (1980) has been used in implementing the ECM scheme into the TOUGH2 code. In terms of the van Genuchten function, the capillary pressure  $P_c$  is expressed in terms of a function of an effective saturation  $S_e$  as

$$P_c(S_e) = \frac{1}{\alpha} \left[ S_e^{-\frac{1}{m}} - 1 \right]^n \quad (5.3.2.1)$$

where the effective saturation is given by

$$S_e = \frac{S_l - S_{lr}}{S_s - S_{lr}} \quad (5.3.2.2)$$

where  $S_l$  is liquid saturation;  $S_{lr}$  is residual liquid saturation;  $S_s$  is saturated saturation;  $\alpha$  ( $\text{Pa}^{-1}$ ),  $n$ , and  $m$ , are empirical fitting parameters, with

$$m = 1 - \frac{1}{n} \quad (5.3.2.3)$$

The liquid phase relative permeability, as a function of effective saturation is given by,

$$k_{rl}(S_e) = \sqrt{S_e} \left[ 1 - \left( 1 - S_e^m \right)^m \right]^2 \quad (5.3.2.4)$$

Relative permeability and capillary pressure for both fracture and matrix data are input through Record "ROCKS" in the TOUGH2 code, and the related modifications in input data are read only in Cards ROCKS.1, ROCKS.1.1, ROCKS.1.2, and ROCKS.1.3 when using the effective continuum approach.

#### a. Permeability Data

(i) In Card ROCKS.1 of "ROCKS"

PER(i) =  $k_m^i$  Absolute continuum matrix permeability ( $m^2$ )  
(i=1,2,3) along the three principal axes or directions.

(ii) In Card ROCKS.1.1 (Col. 51-80, (3E10.4))

PERF(i)=  $k_f^i$  absolute continuum fracture permeability ( $m^2$ )  
(i=1,2,3) along the three principal axes or directions.

leave blank for Col. 51-80 if fractures are treated as isotropic.

(iii) In Card ROCKS.1.2 (I5, 5X, 7E10.4)

IRP= 11 for ECM option.

RP(1)=  $m_m$  of van Genuchten's function, Equation (5.3.2.3), for matrix.

RP(2)=  $S_{lr}$  residual liquid saturation in matrix.

RP(3)=  $m_f$  of van Genuchten's function, Equation (5.3.2.3) for fractures.

RP(4)=  $S_{lr}$  residual liquid saturation in fractures.

RP(5)=  $> 0$   $k_{re} = 1.0 - k_{rl}$   
 $< 0$  using Corey's function for  $k_{re}$ .

RP(6)=  $S_{gr}$  residual gas saturation in matrix.

RP(7)=  $\phi_f$  fracture continuum porosity

#### b. Capillary Pressure Data

(i) In Card ROCKS.1.3 (I5, 5X, 7E10.4)

ICP= 9 for ECM option.

CP(1)=  $m_m$  of van Genuchten's m, Equation (5.3.2.3), for matrix.

CP(2)=  $S_{lr}$  residual liquid saturation in matrix.

CP(3)=  $\alpha_m$  with a unit  $Pa^{-1}$ , van Genuchten's Parameter, Equation (5.3.2.1), for matrix.

CP(4)=  $P_{cmax}$  maximum capillary pressure allowed.

CP(5)=  $S_{lr}$  residual liquid saturation in fractures.

CP(6)=  $m_f$  of van Genuchten's m, Equation (5.3.2.3), for fractures.

CP(7)=  $\alpha_f$  with a unit  $Pa^{-1}$ , van Genuchten's Parameter, Equation (5.3.2.1), for fractures

### Saturated/Unsaturated Flow Module (EOS9)

For the unsaturated/unsaturated flow (Richard's equation) module, the input data and formats are the same as those for the TOUGH2 EOS3 module (Pruess et al., 1966), except the following:

a. One of Record "ROCKS" in the TOUGH2 code, Card ROCKS.1 introduces formation fluid and temperature data with material name "REFCO" with format (A5,5X,5E10), and the five following parameters are defined as

<u>Column</u>	<u>Parameter</u>	<u>Definition</u>
Col. 1-5	REFCO	Rock name
Col: 11-20	$P_{ref}$	Reference gas pressure (Pa) above which the system becomes fully saturated
Col: 21-30	$T_{ref}$	Reference formation temperature (°C)
Col: 31-40	$\rho_l$	Liquid density (kg/m <sup>3</sup> ) at reference condition
Col: 41-50	$\mu_l$	Liquid viscosity (Pa*s) at reference condition
Col: 51-60	$C_l$	Liquid compressibility (Pa <sup>-1</sup> ) at reference condition

b. Only one primary variable, or only one initial condition, needs to be specified for one element block. If two-phase conditions exist, the primary variable to be initialized is water saturation. For single-phase, fully liquid saturated conditions, the primary variable to be initialized is water pressure.

### Radionuclide Transport Module (T2R3D)

For the radionuclide transport module (T2R3D), the input formats are similar to those of the TOUGH2 EOS3 module (Pruess et al., 1966). However, the additional radionuclide transport properties are needed. These radionuclide transport properties are supplied by the second card of "ROCKS", i.e., ROCKS.1.2, with format (5E10.4), as follows:

<u>Column</u>	<u>Parameter</u>	<u>Definition</u>
Col. 1-10	$\alpha_L$	Longitudinal dispersivity (m)
Col: 11-20	$\alpha_T$	Transverse dispersivity (m)
Col: 21-30	$\lambda$	Radioactive decay constant (s <sup>-1</sup> ), defined as $\lambda = \ln(2)/T_{1/2}$
Col: 31-40	$K_d$	Distribution coefficient, $K_d$ (m <sup>3</sup> /kg)
Col: 41-50	$d_m$	Molecular diffusion coefficient in liquid phase (m <sup>2</sup> /s)

The original card ROCKS.1.2 becomes ROCKS.1.3, and the original ROCKS.1.3 becomes ROCKS.1.4 with the same input parameter, respectively. Also, the initial condition for the mass fraction of a radionuclide needs to be specified, which is the third primary variable. The rest of the primary variables are the same as those of the TOUGH2 EOS3 module, and the specification procedure is the same.

## 5.4 User Features

### Single-Phase Gas (EOS1G), Effective Continuum Method (ECM), Saturated/Unsaturated Flow (EOS9) and Radionuclide Transport (T2R3D) Modules

User features for these modules are substantially identical to those described for TOUGH2 in Section 5.4 of Pruess et al. (1996).

## 5.5 Summary

Verification of this phase of the Software Life Cycle, which relates to installation, user documentation, and provision of code demonstration cases, was completed by providing with this package the sample problems described in Appendix C. These problems demonstrate how the user sets up certain types of problems and manipulates various aspects of the code.

## 5.6 Version History

The single-phase Gas (EOS1G), Effective Continuum Method (ECM), Saturated/Unsaturated Flow (EOS9) and Radionuclide Transport (T2R3D) Modules of TOUGH2 are herein qualified for use with TOUGH2 Version 1.11, as transferred to DOE's Energy Science and Technology Software Center (ESTSC) in November 1994 and January 1995. The developers do not anticipate a need for revision to any of these modules. Additional TOUGH2 modules are in use, e.g. a module with hydrodynamic dispersion. These will be released in due course, following more extensive testing, documentation, and some packaging. When they are ready for release, a new version of TOUGH2 (including the single-phase gas, effective continuum method, saturated/unsaturated flow and radionuclide transport modules) will be sent to ESTSC.

## ACKNOWLEDGMENTS

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## APPENDIX A. MASS BALANCES (EOS1G) <sup>1</sup>

The basic mass-balance equations solved by the TOUGH2 single-phase gas module can all be written in the following general form:

$$\frac{d}{dt} \int_{V_n} M^{(\kappa)} dV = \int_{\Gamma_n} \mathbf{F}^{(\kappa)} \cdot \mathbf{n} d\Gamma + \int_{V_n} \mathbf{q}^{(\kappa)} dV \quad (\text{A.1})$$

The integration here is over an arbitrary subdomain  $V_n$  of the flow system under study, which is bounded by the closed surface  $\Gamma_n$ . The quantity  $M$  appearing in the accumulation term denotes mass or energy per unit volume, with  $\kappa = 1$ (air) and  $\kappa = 2$ (water) labeling the mass components.

The general form of the mass accumulation term is

$$M^{(\kappa)} = \phi \sum_{\beta=1}^{NPH} S_{\beta} \rho_{\beta} X_{\beta}^{(\kappa)} \quad (\text{A.2})$$

The total mass of component  $\kappa$  is obtained by summing over all fluid phases  $\beta = 1, \dots, NPH$ .  $S_{\beta}$  is the saturation (volume fraction) of phase  $\beta$ ,  $\rho_{\beta}$  is density of phase  $\beta$ , and  $X_{\beta}^{(\kappa)}$  is the mass fraction of component  $\kappa$  present in phase  $\beta$ .

The mass flux term is a sum over the phases

$$\mathbf{F}^{(\kappa)} = \sum_{\beta=1}^{NPH} X_{\beta}^{(\kappa)} \mathbf{F}_{\beta} \quad (\text{A.3})$$

for  $\kappa = 1, 2$ . Individual phase fluxes are given by a multi-phase version of Darcy's law:

$$\mathbf{F}_{\beta} = -k \frac{k_{r\beta}}{\mu_{\beta}} \rho_{\beta} (\nabla P_{\beta} - \rho_{\beta} \mathbf{g}) \quad (\text{A.4})$$

Here  $k$  tensor is absolute permeability tensor,  $k_{r\beta}$  is relative permeability of phase  $\beta$ ,  $\mu_{\beta}$  is viscosity of phase  $\beta$ , and

$$P_{\beta} = P + P_{c,\beta} \quad (\text{A.5})$$

is the pressure in phase  $\beta$ , which is the sum of the pressure  $P$  of a reference phase, and the capillary pressure of phase  $\beta$  relative to the reference phase.  $\mathbf{g}$  denotes the vector of gravitational acceleration. Gas phase permeability can be specified to depend on pressure, according to the Klinkenberg relationship  $k = k_0(1 + b/P)$ , where  $k_0$  is absolute permeability at high pressure (Klinkenberg, 1941), and  $b$  is the Klinkenberg parameter.

In dealing with the two mass balance equations, only the gas equation is included, and the water phase is treated as a passive phase. Also, the effects of binary diffusion are ignored.

<sup>1</sup> Adapted from TOUGH2 Software Qualification, Pruess et al., (1996).



## APPENDIX B. SPACE AND TIME DISCRETIZATION<sup>2</sup>

The continuum equations (B.1) are discretized in space using the "integral finite difference" method (Edwards, 1972; Narasimhan and Witherspoon, 1976). Introducing appropriate volume averages, we have

$$\int_{V_n} M dV = V_n M_n \quad (\text{B.1})$$

where  $M$  is a volume-normalized extensive quantity, and  $M_n$  is the average value of  $M$  over  $V_n$ . Surface integrals are approximated as a discrete sum of averages over surface segments  $A_{nm}$ :

$$\int_{\Gamma_n} \mathbf{F}^k \cdot \mathbf{n} d\Gamma = \sum_m A_{nm} F_{nm} \quad (\text{B.2})$$

Here  $F_{nm}$  is the average value of the (inward) normal component of  $\mathbf{F}$  over the surface segment  $A_{nm}$  between volume elements  $V_n$  and  $V_m$ . The discretization approach used in the integral finite difference method and the definition of the geometric parameters are illustrated in Figure 19.

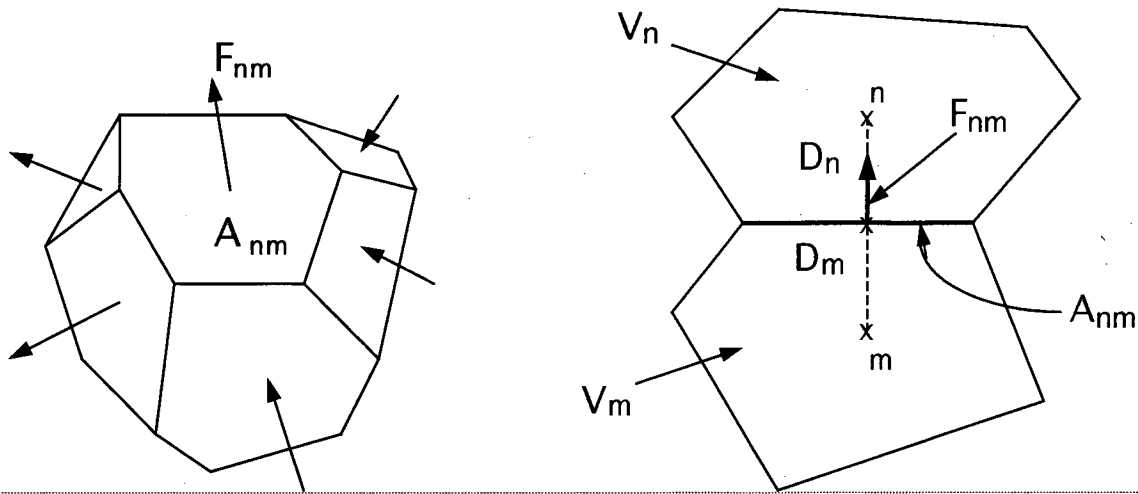


Figure 19. Space discretization and geometry data in the integral finite difference method.

The discretized flux is expressed in terms of averages over parameters for elements  $V_n$  and  $V_m$ . For the basic Darcy flux term, Eq. (A.4), we have

$$F_{\beta, nm} = -k_{nm} \left[ \frac{k_{r\beta} \rho_{\beta}}{\mu_{\beta}} \right]_{nm} \left[ \frac{P_{\beta, n} - P_{\beta, m}}{D_{nm}} - \rho_{\beta, nm} g_{nm} \right] \quad (\text{B.3})$$

<sup>2</sup> Adapted from TOUGH2 report, Pruess (1991).

where the subscripts (nm) denote a suitable averaging at the interface between grid blocks n and m (interpolation, harmonic weighting, upstream weighting).  $D_{nm}$  is the distance between the nodal points n and m, and  $g_{nm}$  is the component of gravitational acceleration in the direction from m to n.

Substituting Eqs. (B.1) and (B.2) into the governing Eq. (A.1), a set of first-order ordinary differential equations in time is obtained.

$$\frac{dM_n^K}{dt} = \frac{1}{V_n} \sum_m A_{nm} F_{nm}^K + q_n^K \quad (B.4)$$

Time is discretized as a first order backward difference, and the flux and sink and source terms on the right hand side of Eq. (B.4) are evaluated at the new time level,  $t^{k+1} = t^k + \Delta t$ , to obtain the numerical stability needed for an efficient calculation of multiphase flow. This treatment of flux terms is known as "fully implicit," because the fluxes are expressed in terms of the unknown thermodynamic parameters at time level  $t^{k+1}$ , so that these unknowns are only implicitly defined in the resulting equations; see e.g. Peaceman (1977). The time discretization results in the following set of coupled non-linear, algebraic equations

$$\begin{aligned} R_n^{\kappa,k+1} &= M_n^{\kappa,k+1} - M_n^{\kappa,k} - \frac{\Delta t}{V_n} \left\{ \sum_m A_{nm} F_{nm}^{\kappa,k+1} + V_n q_n^{\kappa,k+1} \right\} \\ &= 0 \end{aligned} \quad (B.5)$$

where we have introduced residuals  $R_n^{\kappa,k+1}$ . For each volume element (grid block)  $V_n$  there are NEQ equations ( $\kappa = 1, 2, \dots$  NEQ; NEQ = 1), so that for a flow system with NEL grid blocks (B.5) represents a total of NEL • NEQ coupled non-linear equations. The unknowns are the NEL • NEQ independent primary variables  $\{x_i; i = 1, \dots, \text{NEL} \cdot \text{NEQ}\}$  which completely define the state of the flow system at time level  $t^{k+1}$ . These equations are solved by Newton/Raphson iteration, which is implemented as follows. We introduce an iteration index p and expand the residuals  $R_n^{\kappa,k+1}$  in Eq. (B.5) at iteration step p + 1 in a Taylor series in terms of those at index p.

$$\begin{aligned} R_n^{\kappa,k+1}(x_{i,p+1}) &= R_n^{\kappa,k+1}(x_{i,p}) + \sum_i \left. \frac{\partial R_n^{\kappa,k+1}}{\partial x_i} \right|_p (x_{i,p+1} - x_{i,p}) \\ &+ \dots = 0 \end{aligned} \quad (B.6)$$

Retaining only terms up to first order, we obtain a set of NEL • NEQ linear equations for the increments  $(x_{i,p+1} - x_{i,p})$ :

$$- \sum_i \left. \frac{\partial R_n^{\kappa,k+1}}{\partial x_i} \right|_p (x_{i,p+1} - x_{i,p}) = R_n^{\kappa,k+1}(x_{i,p}) \quad (B.7)$$

All terms  $\partial R_n / \partial x_i$  in the Jacobian matrix are evaluated by numerical differentiation. Eq. (B.7) is solved by an iterative sparse matrix solver (Forsyth, 1992). Iteration is continued until the residuals  $R_n^{\kappa,k+1}$  are reduced below a preset convergence tolerance. The selection and switching

of primary variables in a TOUGH2 solution depend on the phase conditions. The variable switching procedure affects the updating for secondary dependent variables but does not affect the equation setup because the equations are still mass and energy conservation equations for each block.

$$\left| \frac{R_{n,p+1}^{\kappa,k+1}}{M_{n,p+1}^{\kappa,k+1}} \right| \leq \epsilon_1 \quad (\text{B.8})$$

$\epsilon_1$  is a convergence tolerance, and the default (relative) convergence criterion is  $\epsilon_1 = 10^{-5}$ . When the accumulation terms are smaller than  $\epsilon_2$  (default  $\epsilon_2 = 1$ ), an absolute convergence criterion is imposed,  $|R_n^{\kappa,k+1}| \leq \epsilon_1 \cdot \epsilon_2$ . Convergence is usually attained in 3 to 4 iterations. If convergence cannot be achieved within a certain number of iterations (default 8), the time step size  $\Delta t$  is reduced and a new iteration process is started.

It is appropriate to add some comments about our space discretization technique. The entire geometric information of the space discretization in Eq. (B.5) is provided in the form of a list of grid block volumes  $V_n$ , interface areas  $A_{nm}$ , nodal distances  $D_{nm}$  and components  $g_{nm}$  of gravitational acceleration along nodal lines. There is no reference whatsoever to a global system of coordinates, or to the dimensionality of a particular flow problem. The discretized equations are in fact valid for arbitrary irregular discretizations in one, two or three dimensions, and for porous as well as for fractured media. This flexibility should be used with caution, however, because the accuracy of solutions depends upon the accuracy with which the various interface parameters in equations such as (B.3) can be expressed in terms of average conditions in grid blocks. A general requirement is that there exists approximate thermodynamic equilibrium in (almost) all grid blocks at (almost) all times (Pruess and Narasimhan, 1985). For systems of regular grid blocks referenced to global coordinates (such as  $r - z$ ,  $x - y - z$ ), Eq. (B.5) is identical to a conventional finite difference formulation (e.g., Peaceman, 1977).

To demonstrate the utility of the newly-implemented TOUGH2 modules and familiarize the user with the input and output formats, four sample problems are provided in this appendix. The user can also use these samples to check the proper installation of these TOUGH2 modules for handling common applications of the codes. The four problems are summarized as follows.

### C-1 Sample Problem 1 - for the single-phase gas flow module (EOS1G)

This is a sample problem for running the EOS1G module. The problem consists of a one-dimensional vertical grid with 99 uniform elements. The input and output files are shown in Figures 20 and 21. As can be seen from Figure 20, the input data format for the EOS1G is identical to that of the TOUGH2 EOS 3 module. This is one-dimensional vertical gas flow under two-phase and non-isothermal conditions. The top boundary element is treated as being at constant gas pressure, liquid saturation, and temperature by specifying a huge volume, and the bottom boundary is treated as a closed boundary by default. The key word "RTSOL" introduces the following two parameter cards for the iterative matrix solver, time stepping and under-relaxation option (see the README file in Appendix D).

```
* 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
3 0.00 0.00
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
3 0.00 0.00
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
3 0.00 0.00
7 .167 .000 .1670E-4 .100E+13 .100E+01
PARAM 123456789012345678901234
5 30005 00051000001 0040 203000 0 2.13e-05
8.640E+06 7.200E+03 7.200E+03 9.80665 3.0
1.00E-05
0.940250000000000E+05 1.100000000000000E+01 2.500000000000000E+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+50
AAA 2 96 1 1.000E+00
AAA99 3 1.000E+00
CONNE
AAA 1AAA 2 97 1 1 3 0.500E+00 0.500E+00 1.000E+00 1.000E+00
INCON -- INITIAL CONDITIONS FOR 99 ELEMENTS AT TIME 0.100000E+14
AAA 1 0.10000000E-01 0.8893899544987E+05 0.1043045016987E+02 0.10000000000000E+02
AAA 2 0.10000000E-01 0.8894966957162E+05 0.1042932329712E+02 0.1020238560150E+02
AAA 3 0.10000000E-01 0.8896033727640E+05 0.1042818349097E+02 0.1040480754828E+02
.
.
.
AAA96 0.10000000E-01 0.8992375231560E+05 0.1006826895250E+02 0.2938271199422E+02
AAA97 0.10000000E-01 0.8993476006888E+05 0.1004967329507E+02 0.2958843768713E+02
AAA98 0.10000000E-01 0.8994779971903E+05 0.1002989124389E+02 0.2979420028375E+02
AAA99 0.10000000E-01 0.90000000000000E+05 0.10010000000000E+02 0.30000000000000E+02
```

Figure 20. Input file for sample problem 1 - EOS1G demonstration.

```

***** VOLUME- AND MASS-BALANCES
***** [KCYC,ITER] = [ 0, 0] ***** THE TIME IS 0.00000E+00 SECONDS, OR
0.00000E+00 DAYS

PHASE VOLUMES IN PLACE
GAS 0.31045E+00 M**3

MASS IN PLACE
GAS 0.32854E+00 KG
*****
*****
AAA99( 1, 1) ST = 0.720000E+04 DT = 0.720000E+04 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 30.000 P = 90000. S
= 0.100000E-01
average inner-iteration/solve = 0.000000000000E+0000
AAA99( 2, 1) ST = 0.144000E+05 DT = 0.720000E+04 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 30.000 P = 90000. S
= 0.100000E-01
average inner-iteration/solve = 0.000000000000E+0000
AAA99( 3, 1) ST = 0.216000E+05 DT = 0.720000E+04 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 30.000 P = 90000. S
= 0.100000E-01
average inner-iteration/solve = 0.000000000000E+0000
AAA99( 4, 1) ST = 0.288000E+05 DT = 0.720000E+04 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 30.000 P = 90000. S
= 0.100000E-01
average inner-iteration/solve = 0.000000000000E+0000
AAA99( 5, 1) ST = 0.360000E+05 DT = 0.720000E+04 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 30.000 P = 90000. S
= 0.100000E-01
average inner-iteration/solve = 0.000000000000E+0000
* INPUT sample for single-phase gas module (eoslg)
OUTPUT DATA AFTER ( 5, 1)-2-TIME STEPS THE TIME IS
0.41667E+00 DAYS
*****
TOTAL TIME KCYC ITER ITERC KON DX1M DX2M DX3M MAX. RES. NER KER
DELTEX
0.36000E+05 5 1 5 2 0.00000E+00 0.00000E+00 0.00000E+00 0.62186E-08 99 1
0.72000E+04
*****
ELEM. INDEX P T SG SL XAIRG XAIRL PSAT PCAP Sf
Sm (PA) (DEG-C) (PA) (PA)
AAA 1 1 0.88939E+05 0.10000E+02 0.43045E+00 0.56955E+00 0.99137E+00 0.10000E+02 0.12270E+04 0.00000E+00
0.43045E+00 0.43045E+00
AAA 2 2 0.88950E+05 0.10202E+02 0.42932E+00 0.57068E+00 0.99125E+00 0.10202E+02 0.12437E+04 0.00000E+00
0.42932E+00 0.42932E+00
AAA 3 3 0.88960E+05 0.10405E+02 0.42818E+00 0.57182E+00 0.99113E+00 0.10405E+02 0.12607E+04 0.00000E+00
0.42818E+00 0.42818E+00
.
.
.
AAA97 97 0.89935E+05 0.29588E+02 0.49673E-01 0.95033E+00 0.97079E+00 0.29588E+02 0.41423E+04 0.00000E+00
0.49673E-01 0.49673E-01
AAA98 98 0.89948E+05 0.29794E+02 0.29891E-01 0.97011E+00 0.97044E+00 0.29794E+02 0.41916E+04 0.00000E+00
0.29891E-01 0.29891E-01
AAA99 99 0.90000E+05 0.30000E+02 0.10000E-01 0.99000E+00 0.97010E+00 0.30000E+02 0.42415E+04 0.00000E+00
0.10000E-01 0.10000E-01
*****

```

Figure 21. Selected output for sample problem 1 - EOSIG demonstration.

## C-2 Sample Problem 2 - for the effective continuum method module

This is a sample problem for running the TOUGH2 EOS3 module using the ECM formulation for fracture/matrix flow. The problem consists of one-dimensional vertical grid with 26 non-uniform elements. The input and output files are shown in Figure 22 and 23. The input data format for the ECM module is the same as that of the standard TOUGH2 EOS3 module, except that both fracture and matrix properties are needed to be input from ROCK.1.2 and ROCK.1.3., as shown in Figure 22.

This is a one-dimensional vertical moisture flow problem under two-phase and isothermal conditions. The top and bottom boundary elements are treated as being at constant gas pressure, liquid saturation, and temperature by specifying a large volume. Also the second element from the top is subject to a constant water infiltration. As can be seen in Figure 23, the last two columns in the selected output present water saturation in fractures and matrix, respectively, for each fracture/matrix element.

```
*input for a 1-d ecm run, 9/17/96
ROCKS
tcw11  2 2480.    0.6200E-010.1600E-180.1600E-180.1600E-18 1.730    935.8
          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
tcw12  2 2480.    0.8200E-010.5400E-150.5400E-150.5400E-15 1.730    935.8
          1.7300    0.2500    0.5750E-110.5750E-110.5750E-11
          11    0.2340    0.1300    0.2236    0.1000E-010.1000E+08    0.2900E-03
          9    0.2340    0.1300    0.1839E-050.1000E+130.1000E-010.2236    0.9770E-03
tcw13  2 2480.    0.2070    0.2200E-160.2200E-160.2200E-16 1.730    826.3
          1.7300    0.2500    0.5750E-110.5750E-110.5750E-11
          11    0.4201    0.3300    0.4370    0.1000E-010.1000E+08    0.2900E-03
          9    0.4201    0.3300    0.1827E-050.1000E+130.1000E-010.4370    0.1230E-02
ptn21  2 2300.    0.4350    0.4000E-120.4000E-120.4000E-12 0.8500    1373.
          0.8500    1.0000
          7    0.2161    0.1000    1.0000
          7    0.2161    0.1000    0.2536E-040.1000E+13 1.0000
ptn22  2 2300.    0.2220    0.2400E-120.2400E-120.2400E-12 0.8500    1373.
          0.8500    1.0000
          7    0.3081    0.1400    1.0000
          7    0.3081    0.1400    0.1603E-040.1000E+13 1.0000
ptn23  2 2300.    0.4060    0.1117E-120.1117E-120.1117E-12 0.8500    1461.
          0.8500    1.0000
          7    0.2438    0.1700    1.0000
          7    0.2438    0.1700    0.4451E-040.1000E+13 1.0000
ptn24  2 2300.    0.4990    0.8800E-130.8800E-130.8800E-13 0.8500    1353.
          0.8500    1.0000
          7    0.2959    0.1000    1.0000
          7    0.2959    0.1000    0.3412E-040.1000E+13 1.0000
ptn25  2 2300.    0.4900    0.1055E-110.1055E-110.1055E-11 0.8500    1353.
          0.8500    1.0000
          7    0.2391    0.1000    1.0000
          7    0.2391    0.1000    0.1384E-030.1000E+13 1.0000
tsw31  2 2480.    0.4800E-010.2614E-120.2614E-120.2614E-12 1.700    848.5
          1.7000    0.4000E-110.4000E-110.4000E-11
          11    0.2066    0.1100    0.2030    0.1000E-010.1000E+08    0.2430E-03
          9    0.2066    0.1100    0.2625E-040.1000E+130.1000E-010.2030    0.1220E-02
tsw32  2 2480.    0.1560    0.1942E-120.1942E-120.1942E-12 1.700    938.3
          1.7000    0.4455E-110.4455E-110.4455E-11
          11    0.2513    0.4000E-010.2493    0.1000E-010.2500E+05    0.2430E-03
          9    0.2513    0.4000E-010.1730E-040.1000E+130.1000E-010.2493    0.9691E-03
tsw33  2 2480.    0.1540    0.7962E-170.7962E-170.7962E-17 1.600    916.7
          1.6000    0.7520E-110.7520E-110.7520E-11
          11    0.2473    0.6000E-010.2443    0.1000E-010.2500E+07    0.2430E-03
          9    0.2473    0.6000E-010.5394E-050.1000E+130.1000E-010.2443    0.2170E-03
tsw34  2 2480.    0.1100    0.1005E-140.1005E-140.1005E-14 2.100    952.9
          2.1000    0.1592E-110.1592E-110.1592E-11
          11    0.3217    0.1800    0.3253    0.1000E-010.2000E+07    0.2430E-03
          9    0.3217    0.1800    0.7721E-060.1000E+130.1000E-010.3253    0.6861E-03
tsw35  2 2480.    0.1300    0.4220E-150.4220E-150.4220E-15 2.100    952.9
          2.1000    0.4000E-110.4000E-110.4000E-11
          11    0.2289    0.8000E-010.2262    0.1000E-010.2000E+07    0.2430E-03
          9    0.2289    0.8000E-010.2429E-050.1000E+130.1000E-010.2262    0.1087E-02
tsw36  2 2480.    0.1120    0.1951E-150.1951E-150.1951E-15 2.100    931.3
          2.1000    0.4000E-110.4000E-110.4000E-11
          11    0.4160    0.1800    0.4160    0.1000E-010.2000E+07    0.2430E-03
          9    0.4160    0.1800    0.5299E-060.1000E+130.1000E-010.4160    0.1220E-02
tsw37  2 2480.    0.3600E-010.3170E-150.3170E-15 1.280    782.8
          1.2800    0.4000E-110.4000E-110.4000E-11
          11    0.3712    0.5000    0.3680    0.1000E-010.1000E+08    0.2430E-03
          9    0.3712    0.5000    0.9912E-060.1000E+130.1000E-010.3680    0.1220E-02
ch1vc  2 2300.    0.2730    0.1600E-110.1600E-110.1600E-11 1.200    1635.
          1.2000    0.7230E-120.7230E-120.7230E-12
          11    0.2210    0.4000E-010.2270    0.1000E-010.1000E+08    0.1110E-03
          9    0.2210    0.4000E-010.7285E-040.1000E+130.1000E-010.2270    0.1220E-02
ch1zc  2 2300.    0.2880    0.5400E-150.5400E-150.5400E-15 1.200    1635.
          1.2000    0.1000E-120.1000E-120.1000E-12
          11    0.3590    0.3600    0.3590    0.1000E-010.1000E+08    0.5250E-04
          9    0.3590    0.3600    0.1900E-060.1000E+130.1000E-010.3590    0.7300E-03
ch2vc  2 2300.    0.3440    0.5500E-130.5500E-130.5500E-13 1.200    1451.
          1.2000    0.7230E-120.7230E-120.7230E-12
```

```

11 0.2232 0.6000E-010.2270 0.1000E-010.1000E+08 0.1110E-03
9 0.2232 0.6000E-010.9800E-040.1000E+130.1000E-010.2270 0.1220E-02
ch3vc 2 2300. 0.3440 0.5500E-130.5500E-130.5500E-13 1.200 1451.
1.2000 0.7230E-120.7230E-120.7230E-12
11 0.2232 0.6000E-010.2270 0.1000E-010.1000E+08 0.1110E-03
9 0.2232 0.6000E-010.9800E-040.1000E+130.1000E-010.2270 0.1220E-02
ch4vc 2 2300. 0.3440 0.5500E-130.5500E-130.5500E-13 1.200 1451.
1.2000 0.7230E-120.7230E-120.7230E-12
11 0.2232 0.6000E-010.2270 0.1000E-010.1000E+08 0.1110E-03
9 0.2232 0.6000E-010.9800E-040.1000E+130.1000E-010.2270 0.1220E-02
ch2zc 2 2300. 0.3320 0.4500E-170.4500E-170.4500E-17 1.200 1451.
1.2000 0.1000E-120.1000E-120.1000E-12
11 0.2251 0.2000 0.2250 0.1000E-010.1000E+08 0.5250E-04
9 0.2251 0.2000 0.3940E-050.1000E+130.1000E-010.2250 0.3466E-03
ch3zc 2 2300. 0.3320 0.4500E-170.4500E-170.4500E-17 1.200 1451.
1.2000 0.1000E-120.1000E-120.1000E-12
11 0.2251 0.2000 0.2250 0.1000E-010.1000E+08 0.5250E-04
9 0.2251 0.2000 0.3940E-050.1000E+130.1000E-010.2250 0.3466E-03
ch4zc 2 2300. 0.2660 0.2110E-160.2110E-160.2110E-16 1.200 1451.
1.2000 0.1000E-120.1000E-120.1000E-12
11 0.4759 0.3300 0.4710 0.1000E-010.1000E+08 0.5250E-04
9 0.4759 0.3300 0.1500E-060.1000E+130.1000E-010.4710 0.7300E-03
pp3vp 2 2300. 0.3220 0.5428E-140.5428E-140.5428E-14 1.560 1509.
1.5600 0.3000E-130.3000E-130.3000E-13
11 0.3002 0.7000E-010.3130 0.1000E-010.1000E+08 0.1110E-03
9 0.3002 0.7000E-010.2412E-040.1000E+130.1000E-010.3130 0.1220E-02
pp2zp 2 2300. 0.2860 0.2694E-150.2694E-150.2694E-15 1.560 1425.
1.5600 0.1000E-120.1000E-120.1000E-12
11 0.3117 0.1800 0.3120 0.1000E-010.1000E+08 0.5250E-04
9 0.3117 0.1800 0.1267E-050.1000E+130.1000E-010.3120 0.7300E-03
bf3vb 2 2300. 0.3220 0.5428E-140.5428E-140.5428E-14 1.560 1509.
1.5600 0.3000E-130.3000E-130.3000E-13
11 0.3002 0.7000E-010.3130 0.1000E-010.1000E+08 0.1110E-03
9 0.3002 0.7000E-010.2412E-040.1000E+130.1000E-010.3130 0.1220E-02
bf2zb 2 2300. 0.2860 0.2694E-150.2694E-150.2694E-15 1.560 1425.
1.5600 0.1000E-120.1000E-120.1000E-12
11 0.3117 0.1800 0.3120 0.1000E-010.1000E+08 0.5250E-04
9 0.3117 0.1800 0.1267E-050.1000E+130.1000E-010.3120 0.7300E-03
tm3vt 2 2300. 0.3220 0.5428E-140.5428E-140.5428E-14 1.560 1509.
1.5600 0.3000E-130.3000E-130.3000E-13
11 0.3002 0.7000E-010.3130 0.1000E-010.1000E+08 0.1110E-03
9 0.3002 0.7000E-010.2412E-040.1000E+130.1000E-010.3130 0.1220E-02
topbd 3 2480. 0.90 .100E-19 .100E-19 .100E-19 1.73 1.e30
0.0 0.0 0.01000 0.25
3 .200 .300 .7 .8
1 .000 .000 1.0
botbd 3 2300. 0.90 .100E-15 .100E-15 .100E-15 1.56 1.e30
0.000 0.250
7 .19 .000 .100E+01
7 .19 .000 .0100E-6 .100E+13 .100E+01

PARAM 123456789012345678901234
4 20005 0005100000000000002030 140 0.00e-05
0.00000E003.15576E15 1.0000E01 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 2 2 8

START
ELEM
TP221 topbd0.1701E+050.0000E+00 171084.80231331.882 1362.640
11221 tcw110.7270E+060.0000E+00 171084.80231331.882 1340.650
12221 tcw120.7270E+060.0000E+00 171084.80231331.882 1296.670
13221 tcw130.1020E+060.0000E+00 171084.80231331.882 1271.680
21221 ptn210.5080E+050.0000E+00 171084.80231331.882 1267.185
22221 ptn210.5100E+050.0000E+00 171084.80231331.882 1264.190
23221 ptn230.5100E+050.0000E+00 171084.80231331.882 1261.190
24221 ptn230.8500E+050.0000E+00 171084.80231331.882 1257.190
25221 ptn250.1710E+060.0000E+00 171084.80231331.882 1249.265
31221 tsw310.6810E+050.0000E+00 171084.80231331.882 1241.824
32221 tsw330.8180E+060.0000E+00 171084.80231331.882 1215.621
33221 tsw330.8180E+060.0000E+00 171084.80231331.882 1167.247
34221 tsw340.2380E+060.0000E+00 171084.80231331.882 1136.005
41221 tsw340.1700E+060.0000E+00 171084.80231331.882 1123.950
42221 tsw340.1020E+060.0000E+00 171084.80231331.882 1115.950
43221 tsw350.1700E+060.0000E+00 171084.80231331.882 1107.950
51221 tsw350.7620E+060.0000E+00 171084.80231331.882 1080.693
52221 tsw360.1140E+070.0000E+00 171084.80231331.882 1025.052
53221 tsw370.3180E+060.0000E+00 171084.80231331.882 982.394
61221 ch1vc0.6370E+060.0000E+00 171084.80231331.882 953.905
62221 ch2vc0.7140E+060.0000E+00 171084.80231331.882 913.750
63221 ch3zc0.1700E+060.0000E+00 171084.80231331.882 887.865
64221 ch4zc0.4340E+060.0000E+00 171084.80231331.882 869.915
65221 pp3vp0.9490E+060.0000E+00 171084.80231331.882 829.000
71221 pp2zp0.1180E+070.0000E+00 171084.80231331.882 765.960
BT221 botbd0.1701E+550.0000E+00 171084.80231331.882 730.830

CONNE
11221TP221 0 0 0 30.2199E+020.1000E-050.1701E+050.1000E+01
1222111221 0 0 0 30.2199E+020.2199E+020.1701E+050.1000E+01
1322112221 0 0 0 30.3000E+010.2199E+020.1701E+050.1000E+01
2122113221 0 0 0 30.1495E+010.3000E-010.1701E+050.1000E+01
2222121221 0 0 0 30.1500E+010.1495E-010.1701E+050.1000E+01
2322122221 0 0 0 30.1500E-010.1500E-010.1701E+050.1000E+01
2422123221 0 0 0 30.2500E-010.1500E+010.1701E+050.1000E+01
2522124221 0 0 0 30.5425E-010.2500E+010.1701E+050.1000E+01
3122125221 0 0 0 30.2016E-010.5425E+010.1701E+050.1000E+01
3222131221 0 0 0 30.2419E-020.2016E+010.1701E+050.1000E+01

```

```

3322132221      0      0      0      30.2419E+020.2419E+020.1701E+050.1000E+01
3422133221      0      0      0      30.7055E+010.2419E+020.1701E+050.1000E+01
4122134221      0      0      0      30.5000E+010.7055E+010.1701E+050.1000E+01
4222141221      0      0      0      30.3000E+010.5000E+010.1701E+050.1000E+01
4322142221      0      0      0      30.5000E+010.3000E+010.1701E+050.1000E+01
5122143221      0      0      0      30.2226E+020.5000E+010.1701E+050.1000E+01
5222151221      0      0      0      30.3338E+020.2226E+020.1701E+050.1000E+01
5322152221      0      0      0      30.9274E+010.3338E+020.1701E+050.1000E+01
6122153221      0      0      0      30.1921E+020.9274E+010.1701E+050.1000E+01
6222161221      0      0      0      30.2094E+020.1921E+020.1701E+050.1000E+01
6322162221      0      0      0      30.4945E+010.2094E+020.1701E+050.1000E+01
6422163221      0      0      0      30.1301E+020.4945E+010.1701E+050.1000E+01
6522164221      0      0      0      30.2791E+020.1301E+020.1701E+050.1000E+01
7122165221      0      0      0      30.3513E+020.2791E+020.1701E+050.1000E+01
BT22171221      0      0      0      30.1000E-050.3513E+020.1701E+050.1000E+01

GENER
11221
INCON -- INITIAL CONDITIONS FOR COM1 1.9265E-037.5610E+04
                26 ELEMENTS AT TIME 0.315576E+16
TP221      0.90000000E+00
      0.8559593484441E+05 0.1099977447220E-02 0.1691997500000E+02
11221      0.23300000E+00
      0.8581577082903E+05 0.1004266213641E+02 0.1739917929925E+02
12221      0.71000000E-01
      0.8625589939344E+05 0.1034155205447E+02 0.1833780898134E+02
13221      0.24300000E+00
      0.8650626263154E+05 0.1038049265031E+02 0.1886475979043E+02
21221      0.53300000E+00
      0.8655146291303E+05 0.1038372088772E+02 0.1896185509870E+02
22221      0.53300000E+00
      0.8658158290425E+05 0.1038928271827E+02 0.1902983673765E+02
23221      0.33400000E+00
      0.8661167221461E+05 0.1039268818603E+02 0.1909787430351E+02
24221      0.33400000E+00
      0.8665179489915E+05 0.1038197078569E+02 0.1918849804234E+02
25221      0.45900000E+00
      0.8673137431040E+05 0.1051704575889E+02 0.1947526816086E+02
31221      0.29000000E-01
      0.8680595591339E+05 0.1049767576962E+02 0.1974920321482E+02
32221      0.12000000E+00
      0.8706867485055E+05 0.1021089006028E+02 0.2034180673995E+02
33221      0.12000000E+00
      0.8755411459354E+05 0.1024104618258E+02 0.2145691246237E+02
34221      0.10000000E+00
      0.8786791591245E+05 0.1009641653951E+02 0.2215325031954E+02
41221      0.10000000E+00
      0.8798906420531E+05 0.1007878579037E+02 0.2237281630220E+02
42221      0.10000000E+00
      0.8806949413613E+05 0.1006646127266E+02 0.2251963971563E+02
43221      0.10200000E+00
      0.8814994990963E+05 0.1015737882676E+02 0.2266699725634E+02
51221      0.10200000E+00
      0.8842429393248E+05 0.1017204116323E+02 0.2317144407397E+02
52221      0.10900000E+00
      0.8898515403583E+05 0.1012655032604E+02 0.2420457907555E+02
53221      0.34000000E-01
      0.8941585167711E+05 0.1019928068219E+02 0.2507191575795E+02
61221      0.21800000E+00
      0.8970360805997E+05 0.1052265440982E+02 0.2592881624689E+02
62221      0.34000000E+00
      0.9010904414734E+05 0.1051795901155E+02 0.2714696078608E+02
63221      0.37200000E+00
      0.9037035107499E+05 0.1002073688852E+02 0.2790720876276E+02
64221      0.26700000E+00
      0.9055158973873E+05 0.1001743089346E+02 0.2833339453246E+02
65221      0.34100000E+00
      0.9096474766642E+05 0.1055639043535E+02 0.2932147459057E+02
71221      0.30300000E+00
      0.9160151369885E+05 0.1027299684212E+02 0.3090246006374E+02
BT221      0.90000000E+00
      0.9199186048050E+05 0.1000100000000E+02 0.3184000000000E+02

```

Figure 22. Input file for sample problem 2 - ECM demonstration.



```

***** VOLUME- AND MASS-BALANCES
***** [KCYC,ITER] = [ 0, 0] ***** THE TIME IS 0.00000E+00 SECONDS, OR
0.00000E+00 DAYS

PHASE VOLUMES IN PLACE
GAS 0.67632E+06 M**3; LIQUID 0.14690E+07 M**3

MASS IN PLACE
GAS 0.69518E+06 KG; LIQUID 0.14647E+10 KG; AIR 0.69841E+06 KG; VAPOR 0.16990E+05 KG; LIQUID WATER
0.14646E+10 KG

*****
****

...ITERATING... AT [ 1, 1] --- DELTEX = 0.100000E-02 MAX. RES. = 0.635638E-06 AT ELEMENT 31221 EQUATION 1
TP221( 1, 2) ST = 0.100000E+02 DT = 0.100000E+02 DX1= -.516152E-04 DX2= 0.914649E-14 T = 16.920 P = 85596. S
= 0.999774E+00

average inner-iteration/solve = 1.000000000000
...ITERATING... AT [ 2, 1] --- DELTEX = 0.175000E+02 MAX. RES. = 0.111236E-05 AT ELEMENT 31221 EQUATION 1
13221( 2, 2) ST = 0.275000E+02 DT = 0.175000E+02 DX1= 0.665260E-01 DX2= -.324891E-06 T = 18.865 P = 86506. S
= 0.380492E+00

average inner-iteration/solve = 1.000000000000
...ITERATING... AT [ 3, 1] --- DELTEX = 0.306250E+02 MAX. RES. = 0.194660E-05 AT ELEMENT 31221 EQUATION 1
13221( 3, 2) ST = 0.581250E+02 DT = 0.306250E+02 DX1= 0.583322E-01 DX2= -.568556E-06 T = 18.865 P = 86506. S
= 0.380492E+00

average inner-iteration/solve = 1.000000000000
...ITERATING... AT [ 4, 1] --- DELTEX = 0.535938E+02 MAX. RES. = 0.340651E-05 AT ELEMENT 31221 EQUATION 1
13221( 4, 2) ST = 0.111719E+03 DT = 0.535938E+02 DX1= 0.461446E-01 DX2= -.994951E-06 T = 18.865 P = 86506. S
= 0.380491E+00

average inner-iteration/solve = 1.000000000000
...ITERATING... AT [ 5, 1] --- DELTEX = 0.937891E+02 MAX. RES. = 0.596128E-05 AT ELEMENT 31221 EQUATION 1
21221( 5, 2) ST = 0.205508E+03 DT = 0.937891E+02 DX1= -.317516E-01 DX2= 0.166343E-05 T = 18.962 P = 86551. S
= 0.383725E+00

average inner-iteration/solve = 1.000000000000

*input for a 1-d ecm run, 9/17/96

OUTPUT DATA AFTER ( 5, 2)-2-TIME STEPS THE TIME IS
0.23786E-02 DAYS

#####
TOTAL TIME KCYC ITER ITERC KON DX1M DX2M DX3M MAX. RES. NER KER
DELTEX 0.20551E+03 5 2 10 2 0.41816E-01 0.29945E-05 0.00000E+00 0.37353E-12 5 2
0.93789E+02

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

TP221 1 0.85596E+05 0.16920E+02 0.99977E+00 0.22553E-03 0.98587E+00 0.13449E-04 0.19264E+04 0.00000E+00
0.22553E-03 0.22553E-03
11221 2 0.85816E-05 0.17399E+02 0.42662E-01 0.95734E+00 0.98546E+00 0.13475E-04 0.19857E+04 -.34591E+05
0.52648E+00 0.95888E+00
12221 3 0.86256E+05 0.18338E+02 0.34155E+00 0.65845E+00 0.98465E+00 0.13527E-04 0.21066E+04 -.24979E+07
0.11473E+00 0.65994E+00
13221 4 0.86506E+05 0.18865E+02 0.38049E+00 0.61951E+00 0.98418E+00 0.13556E-04 0.21773E+04 -.17444E+07
0.12569E-01 0.60430E+00

65221 24 0.90965E+05 0.29321E+02 0.55639E+00 0.44361E+00 0.97158E+00 0.13966E-04 0.40791E+04 -.38148E+06
0.70276E-01 0.42453E+00
71221 25 0.91602E+05 0.30902E+02 0.27300E+00 0.72700E+00 0.96905E+00 0.14007E-04 0.44662E+04 -.17067E+07
0.49072E-01 0.70958E+00
BT221 26 0.91992E+05 0.31840E+02 0.10000E-02 0.99900E+00 0.96746E+00 0.14030E-04 0.47105E+04 -.14299E+07
0.99900E+00 0.99900E+00

#####

```

Figure 23. Selected output for sample problem 2.

### C-3 Sample Problem 3 - for the EOS9 module

This is a sample problem for running the EOS9 module using the dual-permeability approach for fracture/matrix flow. The problem consists of a one-dimensional vertical grid with 45 non-uniform fracture and matrix elements, and the matrix and fracture blocks are subdivided into only one single continuum, respectively, for the vertical fracture/matrix system. This is one-

dimensional vertical moisture flow problem under two-phase and isothermal conditions. The bottom boundary elements are treated as being at constant liquid saturation by specifying a huge volume, and the top element is subject to a constant water infiltration.

The input and output files used are shown in Figures 24 and 25. The input data format for the EOS9 module is similar to that of the standard TOUGH2 EOS3 module, except that one of the "ROCKS" card, which starts with "REFCO", and different initial condition specification, as shown in Figure 24.

```

* input sample for runing the tough2 eos9 module, 9/17/96
ROCKS
REFCO      0.930E+05      25.00
tcwF1      2 2480.      0.5000      0.3626E-110.3626E-110.3626E-11 1.730      935.8
           1.7300      0.0000
           7      0.1827      0.0100      1.0000
           7      0.1827      0.0050      0.5187E-03 .1000E+13 1.0000
tcwM1      2 2480.      0.6200E-010.1600E-180.1600E-180.1600E-18 1.730      935.8
           1.7300
           7      0.2201      0.2000      1.0000
           7      0.2201      0.2000      0.1044E-04 .1000E+13 1.0000
tcwF2      2 2480.      0.5000      0.5750E-110.5750E-110.5750E-11 1.730      935.8
           1.7300
           7      0.2236      0.0100      1.000
           7      0.2236      0.0050      0.9770E-03 .1000E+13 1.0

.
.
.

bf2Mz      2 2300.      0.2860      0.2694E-150.2694E-150.2694E-15 1.560      1425.
           1.5600
           7      0.3117      0.1800      1.0000
           7      0.3117      0.1800      0.1267E-05 .1000E+13 1.000
tm3Fv      2 2300.      0.5000      0.3000E-130.3000E-130.3000E-13 1.560      1509.
           1.5600
           7      0.3130      0.0100E-011.0000
           7      0.3130      0.0010E-010.1220E-02 .1000E+13 1.00
tm3Mv      2 2300.      0.3220      0.5428E-140.5428E-140.5428E-14 1.560      1509.
           1.5600
           7      0.3002      0.7000E-011.0000
           7      0.3002      0.7000E-010.2412E-04 .1000E+13 1.000
topbd      3 2480.      0.90      .100E-19 .100E-19 .100E-19 1.73      1.e30
           0.0      0.0      0.01000      0.25
           3      .200      .300      .7      .8
           1      .000      .000      1.0
botbd      3 2300.      0.90      .100E-15 .100E-15 .100E-15 1.56      1.e30
           0.000      0.250
           7      .19      .000      .100E+01
           7      .19      .000      .0100E-6 .100E+13 .100E+01

.
.
.

PARAM      123456789012345678901234
8 20005      000510000000000002030      140      0.00e-05
0.00000E003.15576E20 1.0000E05      dummy      -9.80665      3.0
1.0000e-5
0.700      00E+00      00.9e5
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

START

ELEME
TP425      topbd0.2125E+550.0000E+00      170700.000235100.000 1346.0000
Fa425      tcwF10.1907E+060.0000E+00      170700.000235100.000 1345.0000
Ma425      tcwM10.1380E+060.0000E+00      170700.000235100.000 1345.0000

.
.
.

Fx425      pp2Fz0.6196E+060.0000E+00      170700.000235100.000 748.2000
Mx425      pp2Mz0.6202E+060.0000E+00      170700.000235100.000 748.2000
BT425      botbd0.2125E+550.0000E+00      170700.000235100.000 731.6000

CONNE
Fa425TP425      30.8800E+000.1000E-050.2125E+050.1000E+01
Fb425Fa425      30.8800E+000.8800E+000.2125E+050.1000E+01
Mb425Ma425      30.8800E+000.8800E+000.2125E+050.1000E+01

.
.
.

Fv425Mv425      10.0000E+000.2697E+000.9700E+06

```

```

Fw425Mw425          10.0000E+000.2697E+000.1013E+07
Fx425Mx425          10.0000E+000.2697E+000.7674E+06

GENER
Fa425                COM1 8.2136E-047.5610E+04

INCON -- INITIAL CONDITIONS FOR 45 ELEMENTS AT TIME 0.116496E+20
TP425                0.90000000E+00
0.10000000000000E-02 0.8580449196486E+05
Fa425                0.50000000E+00
0.4702697286642E+00 0.8571521439055E+05
Ma425                0.62000000E-01
0.9197761767435E+00 0.8571521439055E+05
.
.
.
Fx425                0.50000000E+00
0.2366943158827E+00 0.9171025172783E+05
Mx425                0.28600000E+00
0.9974926259411E+00 0.9171025172783E+05
BT425                0.90000000E+00
0.99900000000000E+00 0.9198465259275E+05

ENDCY

```

*Figure 24. Input file for sample problem 3 - EOS9 demonstration.*

```

***** VOLUME- AND MASS-BALANCES
***** [KCYC,ITER] = [ 0, 0] *****
0.00000E+00 DAYS
PHASE VOLUMES IN PLACE
GAS 0.98387E+07 M**3; LIQUID 0.44416E+07 M**3
LIQUID MASS IN PLACE 0.44290E+10 KG
*****
THE TIME IS 0.00000E+00 SECONDS, OR
*****
...ITERATING... AT [ 1, 1] --- DELTEX = 0.100000E+06 MAX. RES. = 0.197902E-03 AT ELEMENT Mx425 EQUATION 1
...ITERATING... AT [ 1, 2] --- DELTEX = 0.100000E+06 MAX. RES. = 0.336127E-03 AT ELEMENT Fx425 EQUATION 1
Mx425( 1, 3) ST = 0.100000E+06 DT = 0.100000E+06 DX1= -.193790E-03 DX2= 0.000000E+00 T = 25.000 P = 1. S
= 0.997299E+00
average inner-iteration/solve = 1.000000000000
...ITERATING... AT [ 2, 1] --- DELTEX = 0.175000E+06 MAX. RES. = 0.340129E-03 AT ELEMENT Mx425 EQUATION 1
Mx425( 2, 2) ST = 0.275000E+06 DT = 0.175000E+06 DX1= -.330189E-03 DX2= 0.000000E+00 T = 25.000 P = 1. S
= 0.996969E+00
average inner-iteration/solve = 1.000000000000
...ITERATING... AT [ 3, 1] --- DELTEX = 0.306250E+06 MAX. RES. = 0.580293E-03 AT ELEMENT Mx425 EQUATION 1
Mx425( 3, 2) ST = 0.581250E+06 DT = 0.306250E+06 DX1= -.554315E-03 DX2= 0.000000E+00 T = 25.000 P = 1. S
= 0.996414E+00
average inner-iteration/solve = 1.000000000000
...ITERATING... AT [ 4, 1] --- DELTEX = 0.535938E+06 MAX. RES. = 0.976307E-03 AT ELEMENT Mx425 EQUATION 1
Mx425( 4, 2) ST = 0.111719E+07 DT = 0.535938E+06 DX1= -.911741E-03 DX2= 0.000000E+00 T = 25.000 P = 1. S
= 0.995503E+00
average inner-iteration/solve = 1.000000000000
...ITERATING... AT [ 5, 1] --- DELTEX = 0.937891E+06 MAX. RES. = 0.161223E-02 AT ELEMENT Mx425 EQUATION 1
...ITERATING... AT [ 5, 2] --- DELTEX = 0.937891E+06 MAX. RES. = 0.159472E-04 AT ELEMENT Mx425 EQUATION 1
Mx425( 5, 3) ST = 0.205508E+07 DT = 0.937891E+06 DX1= -.147676E-02 DX2= 0.000000E+00 T = 25.000 P = 1. S
= 0.994026E+00
average inner-iteration/solve = 1.000000000000
running the tough2 eos9 module, 9/17/96 * input sample for
0.23786E+02 DAYS
OUTPUT DATA AFTER ( 5, 3)-2-TIME STEPS THE TIME IS
*****
TOTAL TIME KCYC ITER ITERC KON DX1M DX2M DX3M MAX. RES. NER KER
DELTEX
0.20551E+07 5 3 12 2 0.14768E-02 0.00000E+00 0.14768E-02 0.11754E-08 44 1
0.93789E+06
*****
ELEM. INDEX PRES (PA) S(liq) PCAP (PA) K(rel) DIFFUS (m^2/s) Sf Sm
TP425 1 0.93000E+050.10000E-020.00000E+000.00000E+000.00000E+00 0.10000E-02 0.10000E-02
Fa425 2 0.93000E+050.47027E+00-.57052E+050.52647E-050.23893E-07 0.47027E+00 0.47027E+00
Ma425 3 0.93000E+050.91978E+00-.65664E+050.34682E-010.85218E-10 0.91978E+00 0.91978E+00
Fb425 4 0.93000E+050.34341E+00-.43024E+050.17281E-050.99322E-08 0.34341E+00 0.34341E+00
Mb425 5 0.93000E+050.99115E+00-.48924E+050.27090E+000.87118E-05 0.99115E+00 0.99115E+00
Fc425 6 0.93000E+050.62789E-01-.31727E+050.66028E-070.60383E-09 0.62789E-01 0.62789E-01
Mc425 7 0.93000E+050.99794E+00-.31727E+050.76154E+000.81520E-06 0.99794E+00 0.99794E+00
21425 8 0.93000E+050.54876E+00-.47676E+060.54313E-040.22515E-06 0.54876E+00 0.54876E+00
22425 9 0.93000E+050.50640E+00-.40526E+060.25473E-030.81960E-06 0.50640E+00 0.50640E+00
23425 10 0.93000E+050.51556E+00-.33325E+060.29582E-040.28113E-07 0.51556E+00 0.51556E+00
24425 11 0.93000E+050.41507E+00-.34890E+060.43885E-040.23582E-07 0.41507E+00 0.41507E+00
25425 12 0.93000E+050.37033E+00-.33038E+060.13452E-050.12734E-07 0.37033E+00 0.37033E+00
Fi425 13 0.93000E+050.20881E+00-.41400E+060.24981E-080.17906E-09 0.20881E+00 0.20881E+00
Mi425 14 0.93000E+050.51534E+00-.76712E+060.14474E-040.65798E-06 0.51534E+00 0.51534E+00
Fj425 15 0.93000E+050.11737E+00-.73415E+060.37262E-090.73369E-10 0.11737E+00 0.11737E+00
Mj425 16 0.93000E+050.44544E+00-.73540E+060.44121E-040.34449E-06 0.44544E+00 0.44544E+00
Fk425 17 0.93000E+050.27669E+00-.25457E+060.67477E-060.33198E-07 0.27669E+00 0.27669E+00
Mk425 18 0.93000E+050.80775E+00-.25438E+060.12290E-010.12242E-08 0.80775E+00 0.80775E+00
Fl425 19 0.93000E+050.15604E+00-.72587E+050.31593E-060.11295E-08 0.15604E+00 0.15604E+00
Ml425 20 0.93000E+050.89750E+00-.82518E+060.80539E-010.58989E-05 0.89750E+00 0.89750E+00
Fm425 21 0.93000E+050.24110E+00-.12597E+060.64144E-070.10537E-08 0.24110E+00 0.24110E+00
Mm425 22 0.93000E+050.80361E+00-.66294E+060.78343E-020.13567E-06 0.80361E+00 0.80361E+00
Fn425 23 0.93000E+050.22919E+00-.15043E+060.39106E-070.80760E-09 0.22919E+00 0.22919E+00
Mn425 24 0.93000E+050.80417E+00-.66027E+060.79012E-020.13642E-06 0.80417E+00 0.80417E+00
Fo425 25 0.93000E+050.21637E+00-.18405E+060.22264E-070.59648E-09 0.21637E+00 0.21637E+00
Mo425 26 0.93000E+050.80431E+00-.65961E+060.79178E-020.13660E-06 0.80431E+00 0.80431E+00
Fp425 27 0.93000E+050.19443E+00-.26785E+060.77887E-080.33870E-09 0.19443E+00 0.19443E+00
Mp425 28 0.93000E+050.80342E+00-.66382E+060.78125E-020.13542E-06 0.80342E+00 0.80342E+00
Fq425 29 0.93000E+050.37773E-01-.98740E+050.10015E-080.38068E-10 0.37773E-01 0.37773E-01
Mq425 30 0.93000E+050.94570E+00-.69110E+060.28540E+000.46587E-05 0.94570E+00 0.94570E+00
Fr425 31 0.93000E+050.49649E-01-.14710E+060.68939E-090.32173E-10 0.49649E-01 0.49649E-01
Mr425 32 0.93000E+050.96438E+00-.38974E+060.21313E+000.16596E-04 0.96438E+00 0.96438E+00
Fs425 33 0.93000E+050.72516E-01-.15178E+060.67179E-080.57215E-11 0.72516E-01 0.72516E-01
Ms425 34 0.93000E+050.99843E+00-.21613E+060.69325E+000.12933E-03 0.99843E+00 0.99843E+00
Ft425 35 0.93000E+050.45250E+00-.43467E+050.26940E-040.20671E-08 0.45250E+00 0.45250E+00
Mt425 36 0.93000E+050.98294E+00-.42791E+050.17161E+000.53809E-08 0.98294E+00 0.98294E+00
Fu425 37 0.93000E+050.45273E+00-.43390E+050.27071E-040.20726E-08 0.45273E+00 0.45273E+00
Mu425 38 0.93000E+050.96598E+00-.76560E+050.10274E+000.30649E-08 0.96598E+00 0.96598E+00
Fv425 39 0.93000E+050.12266E+00-.14490E+050.73871E-050.42202E-09 0.12266E+00 0.12266E+00
Mv425 40 0.93000E+050.99621E+00-.65604E+060.77027E+000.62831E-05 0.99621E+00 0.99621E+00
Fw425 41 0.93000E+050.18223E+00-.58904E+050.55073E-060.89030E-10 0.18223E+00 0.18223E+00
Mw425 42 0.93000E+050.93471E+00-.34853E+060.12736E+000.58792E-06 0.93471E+00 0.93471E+00
Fx425 43 0.93000E+050.23669E+00-.32875E+050.36896E-050.25741E-09 0.23669E+00 0.23669E+00
Mx425 44 0.93000E+050.99403E+00-.60121E+050.47526E+000.35364E-05 0.99403E+00 0.99403E+00
Bt425 45 0.93000E+050.99900E+00-.14299E+070.39814E+000.12876E-03 0.99900E+00 0.99900E+00

```

Figure 25. Selected output for sample problem 3.

## C-4 Sample Problem 4 - for the radionuclide transport module (T2R3D) module

This is a sample problem for running the T2R3D code for a radionuclide transport simulation. The problem consists of a one-dimensional horizontal grid with 10 uniform elements of  $\Delta x=1$  m. The input and output files for this problem are shown in Figure 26 and 27. The input data format for T2R3D is similar to that of the standard TOUGH2 EOS 3 module, and the only differences are (1) the "ROCKS.1.2" card provides the transport properties for the radionuclide; (2) additional initial and boundary conditions are needed to be specified for the radionuclide, as shown in Figure 26.

This is a one-dimensional radionuclide transport problem under single-phase and isothermal conditions. Both inlet and outlet boundary elements are treated as being at a constant pressure, liquid saturation, radionuclide mass fraction, and temperature by specifying a huge volume. The radionuclide is transported into the system at first by advection, hydraulic dispersion and molecular diffusion from  $t=0$ . Figure 27 shows the mass fraction distributions of the radionuclide at each element at different times.

```

input sample for T2R3D, 1-D dispersive transport, 9/17/96
ROCKS
rock1 3 1600. 1.e+00 .89800E-12 .8980e-12 .8980e-12 2.0000000 1.00e+03
0.000 1.00000
3 0.10 0.05 0.0 0.0e-3 1.00e-10
7 .250 .250 0.0067E-4
.250 .000

START
PARAM 123456789012345678901234
4 20005 0005000000000001002030 0 500 1.00e-05
0.00000E061.72800E06 1.000E+01 2.000e+04junkA 0.00000 3.0
1.000 00E+05 0.00 0.0 25.

TIMES
3
8.6400E04 8.6400E05 1.7280E06

MULTI
3 4 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

GENER
ELEM
A11 1 rock10.5000E+500.1000E+01 0.2500E+000.5000E+00-.5000E+00
A11 2 rock10.5000E+000.1000E+01 0.7500E+000.5000E+00-.5000E+00
A11 3 rock10.5000E+000.1000E+01 0.1250E+010.5000E+00-.5000E+00
A11 4 rock10.5000E+000.1000E+01 0.1750E+010.5000E+00-.5000E+00
A11 5 rock10.5000E+000.1000E+01 0.2250E+010.5000E+00-.5000E+00
A11 6 rock10.5000E+000.1000E+01 0.2750E+010.5000E+00-.5000E+00
A11 7 rock10.5000E+000.1000E+01 0.3250E+010.5000E+00-.5000E+00
A11 8 rock10.5000E+000.1000E+01 0.3750E+010.5000E+00-.5000E+00
A11 9 rock10.5000E+000.1000E+01 0.4250E+010.5000E+00-.5000E+00
A1110 rock10.5000E+500.1000E+01 0.4750E+010.5000E+00-.5000E+00

CONNE
A11 1A11 2 10.2500E+000.2500E+000.1000E+01
A11 2A11 3 10.2500E+000.2500E+000.1000E+01
A11 3A11 4 10.2500E+000.2500E+000.1000E+01
A11 4A11 5 10.2500E+000.2500E+000.1000E+01
A11 5A11 6 10.2500E+000.2500E+000.1000E+01
A11 6A11 7 10.2500E+000.2500E+000.1000E+01
A11 7A11 8 10.2500E+000.2500E+000.1000E+01
A11 8A11 9 10.2500E+000.2500E+000.1000E+01
A11 9A1110 10.2500E+000.2500E+000.1000E+01

INCON
A11 1 0.00000000E-01
1.11574000000000E+05 0.00000000000000E+00 1.00000000000000E-05 0.25000000000000E+02

ENDCY

```

Figure 26. Input file for sample problem 4 - T2R3D demonstration.

```

*****
****
All 2( 1, 2) ST = 0.100000E+02 DT = 0.100000E+02 DX1= 0.998722E+04 DX2= 0.000000E+00 T = 25.000 P = 109987. S
= 0.000000E+00
average inner-iteration/solve = 1.000000000000
All 4( 2, 2) ST = 0.300000E+02 DT = 0.200000E+02 DX1= 0.564381E+03 DX2= 0.000000E+00 T = 25.000 P = 107692. S
= 0.000000E+00
average inner-iteration/solve = 1.000000000000
All 4( 3, 2) ST = 0.700000E+02 DT = 0.400000E+02 DX1= 0.233984E+02 DX2= 0.000000E+00 T = 25.000 P = 107715. S
= 0.000000E+00
average inner-iteration/solve = 1.000000000000
All 4( 4, 2) ST = 0.150000E+03 DT = 0.800000E+02 DX1= 0.515795E+00 DX2= 0.000000E+00 T = 25.000 P = 107716. S
= 0.000000E+00
average inner-iteration/solve = 1.000000000000
All 3( 5, 2) ST = 0.310000E+03 DT = 0.160000E+03 DX1= 0.432134E-02 DX2= 0.000000E+00 T = 25.000 P = 109002. S
= 0.000000E+00
average inner-iteration/solve = 1.000000000000
input sample for T2R3D, 1-D dispersive transport, 9/17/96
OUTPUT DATA AFTER ( 5, 2)-2-TIME STEPS THE TIME IS
0.35880E-02 DAYS
#####
TOTAL TIME KCYC ITER ITERC KON DX1M DX2M DX3M MAX. RES. NER KER
DELTEX
0.31000E+03 5 2 10 2 0.66078E-02 0.00000E+00 0.58071E-08 0.10673E-14 3 1
0.16000E+03
#####
ELEM. INDEX P T SG SL XAIRG XAIRL PS.or.X3 PCAP Sf
Sm (PA) (DEG-C)
All 1 1 0.11157E+06 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.00000E+00 0.10000E-04 0.00000E+00
0.10000E+01 0.10000E+01
All 2 2 0.11029E+06 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.00000E+00 0.11262E-07 0.00000E+00
0.10000E+01 0.10000E+01
All 3 3 0.10900E+06 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.00000E+00 0.85872E-11 0.00000E+00
0.10000E+01 0.10000E+01
All 4 4 0.10772E+06 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.00000E+00 0.56565E-14 0.00000E+00
0.10000E+01 0.10000E+01
All 5 5 0.10643E+06 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.00000E+00 0.34913E-17 0.00000E+00
0.10000E+01 0.10000E+01
All 6 6 0.10514E+06 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.00000E+00 0.20895E-20 0.00000E+00
0.10000E+01 0.10000E+01
All 7 7 0.10386E+06 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.00000E+00 0.12318E-23 0.00000E+00
0.10000E+01 0.10000E+01
All 8 8 0.10257E+06 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.00000E+00 0.72085E-27 0.00000E+00
0.10000E+01 0.10000E+01
All 9 9 0.10129E+06 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.00000E+00 0.42028E-30 0.00000E+00
0.10000E+01 0.10000E+01
All 10 10 0.10000E+06 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.00000E+00 0.24467E-83 0.00000E+00
0.10000E+01 0.10000E+01
#####

```

Figure 27. Selected output for sample problem 4.

## APPENDIX D. TOUGH2 MODULES READ.ME FILE

```

*****NEWLY IMPLEMENTED TOUGH2 MODULE, September 1996 *****
***** (1) EOS1G Module *****
***** (2) ECM Module *****
***** (3) EOS9 Module *****
***** (4) T2R3D Module *****
*****

```

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

.....  
.....Update 9/96.....  
.....

This flyer contains brief instructions for installing and running the TOUGH2 code with the newly implemented modules.

TOUGH2 with the new modules is distributed with specifications as follows:

The program is available on 3.5" high-density diskettes, written either in PC-DOS format, or according to specifications of IBM RISC System/6000 workstations. The distribution includes the following 26 files.

- ```

*****

```
- (1) read.me - the file you're reading
  - (2) t2cgn2.f - contains the main program of TOUGH2, with PARAMETER statements for flexible dimensioning of all major arrays, and initialization of disk files; also includes a revised version of subroutine LINEQ that calls a set of iterative sparse matrix solver routines; t2cgn2.f was created by modifying the program module t2cg1.f of the previous version of TOUGH2 (Version 1.11, January 1994);
  - (3) meshmn.f - module with internal mesh generation facilities
  - (4) eos3ecm.f - equation of state for water/air of the TOUGH eos3 with ECM option (similar to TOUGH)
  - (5) eos9ecm.f - equation of state for water/air with air treated as a passive phase and ECM option
  - (6) eos32l.f - equation of state for water, air and radionuclide
  - (7) eos1g.f - equation of state for water/air with water treated as a passive phase
  - (8) t2fecm.f - modified to include ECM option from t2f.f of TOUGH2 Version 1.11; it reads input data, initializes arrays and parameters, sets up the 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
  - (9) t2f2l2.f - similar to t2fecm.f with ECM option used in the T2R3D module
  - (10) t2fecm1g.f - similar to t2fecm.f with ECM option used in the eos1g module

- (11) inter.f interface with and an iterative sparse matrix solver for block matrices (Copy Righted)
- (12) relpecm.f evaluating relative permeability with ECM option
- (13) relp1g.f evaluating relative permeability with ECM option for eos1g
- (14) pcapecm.f evaluating capillary pressure with ECM option
- (15) pcapgen.f generating saturation and capillary pressure tables for ECM option
- (16) sndsaf.f computing time subroutine using the FTN77 Fortran compiler by Salford Software Ltd (December, 1994).
- (18) seconddec.f computing time subroutine using a Digital/ Alpha Station 200 computer and a Fortran 90 compiler as
- (19) corder.f subroutine to sort indexes of all connections for each elements, used in T2R3D
- (20) diffd.f subroutine to calculate hydraulic dispersion and molecular diffusion tensor, used in T2R3D
- (21) gradx.f subroutine to calculate concentration gradients, used in T2R3D
- (22) TOUGH2.PRM Parameter 'INCLUDE' file to set up dimensions of arrays used in the TOUGH2 code.

In addition there are four input files for sample problems.

- (23) reos1g.dat - input file for sample problem 1 (eos1g demonstration)
- (24) recm.dat - input file for sample problem 2 (ECM option)
- (25) reos9.dat - input file for sample problem 3 (eos9 demonstration)
- (26) rt2r3d.dat - input file for sample problem 4 (T2R3D demonstration)

\*\*\*\*\*

Source codes for the different TOUGH2 modules of the PC versions

The TOUGH2 ECM Module:

t2cgn2.f  
 t2fecm.f  
 meshmn.f  
 eos3ecm.f  
 relpecm.f  
 inter.f  
 pcapecm.f  
 pcapgen.f  
 sndsaf.f

The TOUGH2 EOS1G Module:



t2cgn2.f  
t2fecm1g.f  
meshmn.f  
eos1g.f  
relp1g.f  
inter.f  
pcapecm.f  
pcapgen.f  
sndsaf.f

The TOUGH2 EOS9 Module:

t2cgn2.f  
t2fecm9.f  
meshmn.f  
eos9ecm.f  
relpecm.f  
inter.f  
pcapecm.f  
sndsaf.f

The T2R3D Module:

t2cgn2.f  
t2f2l2.f  
meshmn.f  
eos32l.f  
relpecm.f  
inter.f  
pcapecm.f  
pcapgen.f  
sndsaf.f  
gradx.f  
diffd.f  
corder.f

## COMPILATION

---

Compilation of the above TOUGH2 modules is in general computer and compiler dependent. For example, the following compilation is carried out on a Digital/Alphas Station 200 computer using a Fortran 90 compiler as

### COMPILATION:

```
f90 -c t2cgn2.f meshmn.f eos3ecm.f t2fecm.f inter.f \  
relpecm.f pcapecm.f pcapgen.f seconddec.f
```

### LINKING:

```
f90 -c t2ecm.exe t2cgn2.o meshmn.o eos3ecm.o t2fecm.o inter.o \  
relpecm.o pcapecm.o pcapgen.o seconddec.o
```

### EXECUTION

t2ecm

input data file

output file.

The additional parameter specification for the new TOUGH2 modules:

---

The above four new TOUGH2 modules use a set of sparse, iterative matrix solvers, developed and copyrighted by Peter A. Forsyth at the University of Waterloo. Therefore, the original options in the TOUGH2 Version 1.11, pertaining to the solvers of MA28 or T2CG1, a package of conjugate gradient solvers are not applied to these four new modules.

The additional parameter specification for these four new modules are:

"RTSOL" introduces parameters for solvers, time stepping and underrelaxation option. The Key word, RTSOL is followed by two parameter cards as:

Col. 1-5

RTSOL

Card RTSOL.1 with format (2e10.4,6i5) for solver parameters

Col. 1-10 11-20 21-25 26-30 31-35 36-40 41-45 46-50

prec rtol info iplvl nitmx nort kacc iredb

where

prec = convergence checking parameter for the residual reduction stopping criteria, and default value is 1.0e-6.

rtol = convergence checking parameter, if the change in two successive iterations for any variable is less than for the residual reduction  $rtol \cdot (\text{Newton iteration tolerance})$  then convergence is assumed. Default value is 0.1.

stopping criteria, default value is 1.0e-6.

info: detailed information printout index

INFO=0, NO INFORMATION  
INFO=1, DETAILED STORAGE INFORMATION  
INFO=2, STORAGE AND RESIDUAL INFORMATION

iplvl: level of incomplete factorization. Higher levels of iplvl allow more fine-in the incomplete factorization, and hence a more accurate decomposition of the matrix, but requiring more work per iteration. iplvl=1 re recommended.

nitmx: Max. number of solver internal iterations, recommended value is 30.

nort: Number of orthogonal vectors for ORTHOMIN, and GMRES accelerations, default value is 15.

kacc: Acceleration options,

KACCEL=0 ORTHOMIN  
KACCEL=1 CGS  
KACCEL=2 CGSTAB  
KACCEL=3 GMRES.

iredb: Flag for red-black ordering,

IREDB=0 ATTEMPT RED-BLACK ORDERING (RECOMMENDED)  
IREDB=1 DO NOT ATTEMPT RED-BLACK ORDERING

Card RTSOL.2 with format (7e10.4,i10) for time stepping and underrelaxation

Col. 1-10 11-20 21-25 26-30 31-35 36-40 41-45 46-50

dtmin dtmax dstnom dxtnom tmlfrc relxsn relxrn icoley

where

dtmin: Minimum time step size (s).

dtmax: Maximum time step size (s).

dstnom: Max. allowable saturation changes/time step (default=0.2)

dxtnom: Max. allowable mass fraction changes/time step (not used).

tmlfrc: Maximum time step multiplier (default=5).

relxsn: Relaxation saturation norm (default=0.2).

relxrn: Relaxation mass fraction norm (not used).

icoley: Flag for relaxation options,

ICOLEY=0 NO UNDERRELAXATION

ICOLEY=1 USING COOLEY UNDERRELAXATION SCHEME

ICOLEY=2 USING UNDERRELAXATION SCHEM BASED ON SAT. NORM.

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

.....

.....Update 9/96.....

.....

## APPENDIX E.

## NOMENCLATURE

|                  |                                                                                                              |
|------------------|--------------------------------------------------------------------------------------------------------------|
| A                | area, $m^2$                                                                                                  |
| b                | Klinkenberg parameter, Pa                                                                                    |
| B                | effective vapor diffusion strength parameter, replaces the group $\phi S_g \tau$ in Eq. (A.7), dimensionless |
| C                | specific heat, $J/kg \cdot ^\circ C$                                                                         |
| d                | penetration depth for heat conduction, m                                                                     |
| D                | diffusion coefficient, $m^2/s$                                                                               |
| $d_m$            | distance, m                                                                                                  |
| DELX             | small increments of primary variables for computing numerical derivatives                                    |
| DX               | increments of primary variables during Newton-Raphson iteration                                              |
| f                | diffusive flux, $kg/m^2 \cdot s$                                                                             |
| f <sub>VPL</sub> | vapor pressure lowering factor, dimensionless (Eq. A.9)                                                      |
| F                | mass or heat flux, $kg/m^2 \cdot s$ or $W/m^2$                                                               |
| g                | gravity acceleration, $m/s^2$                                                                                |
| h                | specific enthalpy, $J/kg$                                                                                    |
| i                | index of primary thermodynamic variable                                                                      |
| J                | Jacobian matrix                                                                                              |
| k                | intrinsic permeability, $m^2(10^{-12} m^2 \approx 1 \text{ darcy})$                                          |
| $k_d$            | equilibrium constant                                                                                         |
| $k_r$            | relative permeability, dimensionless                                                                         |
| K                | thermal conductivity, $W/m \cdot ^\circ C$                                                                   |
| $K_H$            | Henry's constant, Pa                                                                                         |
| m                | index of volume element (grid block)                                                                         |
| $m_{air}$        | molecular weight of air                                                                                      |
| $m_{H_2O}$       | molecular weight of water                                                                                    |
| $m_l$            | molecular weight of liquid                                                                                   |
| M                | accumulation term in mass or energy balance equation, $kg/m^3$ or $J/m^3$                                    |
| n                | index of volume element (grid block)                                                                         |
| <b>n</b>         | unit vector                                                                                                  |
| N                | index of volume element (grid block)                                                                         |
| NB               | number of secondary parameters other than mass fractions in PAR array (usually NB = 6)                       |
| NBK              | NB + NK                                                                                                      |
| NEL              | number of volume elements (grid blocks) in flow domain                                                       |
| NEQ              | number of balance equations per volume element; NEQ = NK1 or NEQ = NK                                        |
| NK               | number of mass components present                                                                            |
| NK1              | NK + 1                                                                                                       |
| NLOC             | storage location after which primary variables start for grid block N; NLOC = (N - 1)*NK1                    |
| NLOC2            | storage location after which secondary parameters start for grid block N; NLOC2 = (N - 1)*(NEQ + 1)*NSEC     |
| NPH              | number of phases                                                                                             |
| NSEC             | number of secondary parameters per volume element; NSEC = NPK*NBK + 2                                        |
| p                | index in Newton-Raphson iteration                                                                            |
| P                | pressure, Pa                                                                                                 |
| $P_{a.e.}$       | air entry pressure, Pa                                                                                       |
| $P_c$            | capillary pressure, Pa                                                                                       |

|                         |                                                                                  |
|-------------------------|----------------------------------------------------------------------------------|
| $P_{\text{sat}}$        | saturated vapor pressure, Pa                                                     |
| $q$                     | volumetric sink or source rate, $\text{kg/m}^3\cdot\text{s}$ or $\text{W/m}^3$   |
| $r$                     | radius, m                                                                        |
| $R$                     | residuals in mass or energy balance equations, $\text{kg/m}^3$ or $\text{J/m}^3$ |
| $R$                     | universal gas constant, $8314.56 \text{ J/}^\circ\text{C}\cdot\text{mole}$       |
| $S$                     | saturation (void fraction occupied by a fluid phase), dimensionless              |
| $t$                     | time, s                                                                          |
| $T$                     | temperature, $^\circ\text{C}$                                                    |
| $u$                     | specific internal energy, $\text{J/kg}$                                          |
| $v$                     | velocity component                                                               |
| $\mathbf{v}$            | velocity vector                                                                  |
| $V$                     | volume, $\text{m}^3$                                                             |
| $x$                     | distance, m                                                                      |
| $x, X$                  | primary thermodynamic variable                                                   |
| $x_{\beta}^{(\kappa)}$  | mol fraction of component $\kappa$ in phase $\beta$                              |
| $X_{\beta}^{(\kappa)}$  | mass fraction of component $\kappa$ in phase $\beta$                             |
| $z = \log[r/(t)^{1/2}]$ | similarity variable for cylindrical flow geometry                                |

### Greek

|              |                                              |
|--------------|----------------------------------------------|
| $\beta$      | phase index ( $\beta = \text{liquid, gas}$ ) |
| $\epsilon_1$ | convergence tolerance                        |
| $\theta$     | thermal diffusivity, $\text{m}^2/\text{s}$   |
| $\kappa$     | component index                              |
| $\rho$       | density, $\text{kg/m}^3$                     |
| $\Gamma$     | area, $\text{m}^2$                           |
| $\phi$       | porosity, dimensionless                      |
| $\tau$       | tortuosity factor, dimensionless             |
| $\mu$        | viscosity, $\text{Pa}\cdot\text{s}$          |

### Subscripts

|               |              |
|---------------|--------------|
| $a$           | air          |
| $\beta$       | phase        |
| $c$           | capillary    |
| $f$           | fracture     |
| $g$           | gas          |
| $i$           | initial      |
| $l$ or $\ell$ | liquid       |
| $m$           | matrix       |
| $r$           | relative     |
| $R$           | rock         |
| $v$           | vapor        |
| $d$           | distribution |

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