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Design Document for: TOUGH2 V1.1MEOS9NT V2.0

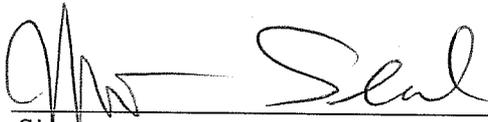
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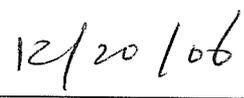
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1. INTRODUCTION

1.1 PURPOSE

This software design document concerns TOUGH2 V1.11MEOS9NT V2.0, a modification of the TOUGH2 V1.11MEOS9NT V1.0 code (Pruess et al., 1999) for the simulation of transport of solutes and/or colloids in porous and fractured media. The modifications are made to allow (a) dynamic memory allocation that eliminates the need to redimension the code to handle different size problems, (b) handling of grids with 8-character cell names that make possible the solution of very large problems, and (c) improved capabilities to describe colloid and colloid-assisted transport.

EOS9NT is a TOUGH2 module for the simulation of flow and transport of an arbitrary number n of tracers (solutes and/or colloids) in the subsurface. The module first solves the Richards equation, which describes saturated or unsaturated water flow in subsurface formations, and obtains the flow regime. A second set of transport equations, corresponding to the n tracers/colloids, is then solved sequentially. The very low concentrations of the n tracers are considered to have no effect on the density or viscosity of the liquid phase, thus making possible the decoupling of the transport from the flow equations. The n tracer transport equations account for sorption, radioactive decay, advection, hydrodynamic dispersion, molecular diffusion, filtration (for colloids only), first-order chemical reactions, and colloid-assisted tracer transport. EOS9NT V2.0 can describe the transport of all colloid classes. These include: Class I colloids (involving true radioactive colloids formed when solute concentration exceeds the species solubility, or waste form colloids formed from spallation of a solid radioactive substances), Class II (pseudocolloids such as clays and oxides, onto which solute radionuclides or other non-radioactive contaminants have sorbed irreversibly), Class III colloids (pseudocolloids onto which solute radionuclides or other non-radioactive contaminants sorbed reversibly), and Class IV colloids (including all non-radioactive true colloids or pseudocolloids not involved in colloid-assisted transport). A total of $n-1$ daughter products of radioactive decay or of a chemical reaction chain can be tracked.

EOS9NT can handle gridblocks of irregular geometry in 3-D domains, and offers the option of a Laplace space formulation of the transport equations (in addition- to conventional time-stepping) after the flow field becomes time-invariant. The Laplace transform formulation option eliminates the need for time discretization and the problems stemming from the treatment of the time derivatives in the transport equations, and yields solutions semi-analytical in time. An unlimited time step size is thus possible without loss of accuracy.

This design has been developed to meet the requirements of the software project's Requirements Document [10065-RD-1.11MEOS9NTV2.0-01] for TOUGH2 V1.11MEOS9NT V2.0 (hereafter abbreviated as EOS9NT V2.0). The software is to be used for numerical simulation predictions of radionuclide transport under ambient conditions at the proposed Yucca Mountain High Level Radioactive Waste Repository.

This document specifies the EOS9NT V2.0 software design based on an explicitly articulated set of requirements. More specifically, it addresses the following aspects of the design:

Major Components—As they relate to the requirements.

Technical Description—In terms of theoretical basis, mathematical model, control flow, data flow, control logic, and data structure.

Input Range—In terms of allowable or defined range of values.

Output Range—In terms of allowable or defined range of values.

Test Plan—For validating the software.

1.2 SOFTWARE IDENTIFICATION

This document contains the design of the TOUGH2 V1.11MEOS9NT V2.0 identified on the title page.

The Software Configuration Control Request (SCCR) (Software Tracking Number [STN]: [10065-DD-1.11MEOS9NTV2.0-01]) specifies the plan used to produce this document.

TOUGH2 V1.11MEOS9NT V2.0 Requirement Document (Document ID: [10065-RD-1.11MEOS9NTV2.0-01]) specifies the requirements that the design implements.

1.3 DEFINITIONS

- **Dynamic Memory Allocation** is the allocation of memory storage for use in a computer program during the runtime of that program. It is a way of distributing ownership of limited memory resources among many pieces of data and code. A dynamically allocated object remains allocated until it is deallocated explicitly.

1.4 TRACEABILITY

The Requirements Traceability Matrix (Document ID: 10065-DD-1.11MEOS9NTV2.0-01) documents the relationships between the following:

- Design Elements (as specified in section 2) and Requirements (as specified in the RD)
- Test Cases (as specified in subsection 5.2) and Design Elements (as specified in section 2)
- Test Cases (as specified in subsection 5.2) and Requirements (as specified in the RD).

2. DESIGN COMPONENTS

The components involved in this software are FORTRAN90/95 subroutines. These accomplish all the basic requirements.

Note: The presence of the asterisk (*) indicates presence of a subroutine of the same name in the standard TOUGH2 code.

DC ID	Req ID	Design Component
DC-01	FR-02 FR-03 DCR-01 AR-01 ER-01 ER-02 ER-03	<p>T2_Main.f90</p> <p>This module includes the main program, and timing and solution subroutines. It is essentially the same as that in standard TOUGH2 V1.6 (STN: 10007-1.6-01), the only modification being the use of dynamic memory allocation rather than direct array dimensioning. It includes the following components (programs and routines):</p> <ol style="list-style-type: none"> (1) TOUGH2 main (*): a high-level executive routine (2) IO (*): routine to read input file (3) FLOP (*): routine to calculate number of significant digits for floating point processing. Assign default for dfac, and print appropriate warning when machine accuracy is insufficient (4) SECOND (*): routine for CPU time function (5) LINEQ (*): routine to call linear equation solver (6) LUBAND(*): routine to use direct banded matrix solver using LU decomposition
DC-02	FR-02	<p>T2_AllocM.f90</p> <p>Dynamic memory allocation occurs within this new module that includes the following routines:</p> <ol style="list-style-type: none"> (1) Allocate_Mem (2) Allocate_MemML
DC-03	FR-02 FR-03 DCR-01	<p>T2_Mesh.f90</p> <p>This module includes the grid creation subroutines. It is essentially the same with that in standard TOUGH2 V1.6 (STN 10007-1.6-01), the only modification being the use of dynamic memory allocation rather than direct array dimensioning. It includes the following components (programs and routines):</p> <ol style="list-style-type: none"> (1) MESHM (*): this is the executive routine for the *meshmaker* module (2) RZ2d (*) (3) WRZ2D (*) (4) PRZ2D (*)

		<p>(5) GXYZ (*) (6) PCAR (*) (7) MINC (*) (8) PART (*) (9) GEOM (*) (10) PROX (*) (11) INVER (*) (12) MINCME (*) (13) ONOMA (*)</p>
DC-04	FR-07 DCR-01	<p>ma28.f90 This module involves a direct matrix solver, and remains completely unchanged, i.e., it is identical to that used in standard TOUGH2.</p>
DC-05	FR-07 DCR-01	<p>T2_Solv.f90 This module involves a package of iterative and direct matrix solvers, and remains completely unchanged, i.e., it is identical to that used in standard TOUGH2 V1.6 (STN 10007-1.6-01).</p>
DC-06	FR-01 FR-04 FR-05 FR-06 DCR-01	<p>T2_EOS9NT.f90 This module includes the subroutines that are involved in tracer transport simulations. It includes the following routines and functions:</p> <ol style="list-style-type: none"> (1) INPUT (*): routine reading all data provided through the input file (2) RFILE (*): routine reading input data from disk files, which are either provided by the user, or are internally generated in subroutine input (3) CUM_DF: routine for computation of the colloid accessibility factor of colloid into media with lognormally-distributed pore sizes (4) DLOGNR: routine to calculate lognormally-distributed pore sizes (5) DQAGPE: routine to approximate a given definite integral $I = \text{Integral of } F \text{ over } (A, B)$, hopefully satisfying the accuracy claim: $\text{ABS}(I - \text{RESULT}) \leq \text{LE.MAX}(\text{EPSABS}, \text{EPSREL} * \text{ABS}(I))$. Break points of the integration interval, where local difficulties of the integrand may occur (e.g. singularities or discontinuities) are provided by the user (6) DQELG: The routine determines the limit of a given sequence of approximations, by means of the Epsilon algorithm of P.Wynn. An estimate of the absolute error is also given. The condensed Epsilon table is computed. Only those elements needed for the

		<p>computation of the next diagonal are preserved</p> <p>(7) DQK61: routine to compute $i = \text{integral of } f \text{ over } (a,b)$ with error estimate, $j = \text{integral of } dabs(f) \text{ over } (a,b)$</p> <p>(8) DQPSRT: This routine maintains the descending ordering in the list of the local error estimated resulting from the interval subdivision process. At each call two error estimates are inserted using the sequential search method, top-down for the largest error estimate and bottom-up for the smallest error estimate.</p> <p>(9) DIMACH:</p> <p>(10) EOS (*): routine performing phase transition diagnostic and computing all thermophysical properties needed for saturated/unsaturated flow of water</p> <p>(11) MULTI (*): SET UP THE COUPLED LINEAR EQUATIONS ARISING AT EACH ITERATION STEP</p> <p>(12) FINDS (*): routine to find gas saturation for specified capillary pressure</p> <p>(13) OUT (*): routine generating flow-related printout</p> <p>(14) WRISAV (*): routine generating a file *save* to be used for restarting</p> <p>(15) RELP (*): routine to calculate Relative Permeability</p> <p>(16) PCAP (*): routine to calculate capillary pressure</p> <p>(17) INTP1 (*):</p> <p>(18) ELINDX: routine to determine the positioning arrays ia and ja which identify the locations of the neighbors</p> <p>(19) SORT: routine to sort the vector iar in ascending order</p> <p>(20) UNITV: routine for sorting the connection indices of the elements and for calculating the unit vectors at the centers of the two elements of a connection</p> <p>(21) DTNSOR: routine for determining darcy velocities and calculating the dispersion tensor</p> <p>(22) VELWTM: routine to calculate the dispersion tensor</p> <p>(23) GRADX: routine for calculating averaged grad (x) along the connections/interfaces n</p> <p>(24) BALLA (*): routine performing volume- and mass-balances</p> <p>(25) COURNT: routine determining max allowable dt_t from grid courant numbers</p> <p>(26) TCYCIT: executive routine for timestepping in the tracer equations</p> <p>(27) QTRACR: routine computing all terms arising from sinks and sources in the tracer equation</p> <p>(28) TMULTI: routine for setting up the linear equation(s) of solute transport</p> <p>(29) TOUT: routine generating printout of tracer-related data</p> <p>(30) SI_TOUT: routine generating printout of tracer-related data</p> <p>(31) TKINFA: function for determining the colloid kinetic factor</p>
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		<p>coefki in the laplace space - stehfest algorithm</p> <p>(32) T_SOFI: routine for determining sorption onto pseudocolloids</p> <p>(33) XB_COMP: routine to compute the tracer mass fractions at the boundaries</p> <p>(34) C_FACT: function to compute the fracture concentration</p> <p>(35) LQTRCR: routine computing all terms arising from sinks and sources in the laplace formulation of the tracer equation (stehfest algorithm)</p> <p>(36) LGRADX: outline for calculating averaged grad (x) contributions in the laplace space along the connections/interfaces n</p> <p>(37) LPACON: function for determining the parent contribution in daughter generation in the laplace space - dehoog algorithm</p> <p>(38) XS_LAPL: function for determining the laplace space concentration of radioactively decaying species</p> <p>(39) LKINFA: function for determining the colloid kinetic factor coefki in the laplace space - stehfest algorithm</p> <p>(40) L_SOFI: routine for determining sorption onto pseudocolloids</p> <p>(41) LMULTI: routine for setting up the linear equation(s) in the laplace formulation of solute transport (stehfest algorithm)</p> <p>(42) LCYCIT: executive routine for solving the tracer equations in the laplace space - stehfest algorithm</p> <p>(43) CYCIT (*): executive routine for marching in time in the flow equation</p> <p>(44) HCYCIT: executive routine for solving the tracer equations IN THE LAPLACE SPACE - DeHOOG ALGORITHM</p> <p>(45) HQTRCR: routine computing all terms arising from sinks and sources in the laplace formulation of the tracer equation (dehoog algorithm)</p> <p>(46) HMULTI: routine for setting up the linear equation(s) in the laplace formulation of solute transport (dehoog algorithm)</p> <p>(47) HTOUT: routine generating printout of tracer-related data when the dehoog formulation is employed</p> <p>(48) SI_HTOUT: routine generating printout of tracer-related data when the dehoog formulation is employed</p> <p>(49) HPACON: function for determining the parent contribution in daughter generation in the laplace space - dehoog algorithm</p> <p>(50) XH_LAPL: function for determining the laplace space concentration of radioactively decaying species</p> <p>(51) HKINFA: function for determining the colloid kinetic factor coefki in the laplace space - dehoog algorithm</p> <p>(52) H_SOFI: routine for determining sorption onto pseudocolloids</p> <p>(53) PSI_SET: routine to compute the transformed mass fraction in the laplace-space using the dehoog method</p> <p>(54) HOOG_1: routine to numerically invert the laplace space solution using the dehoog method</p>
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		(55) HOOG_2: routine to numerically invert the laplace space solution using the dehoog method (56) XT_HOOG: routine to compute decaying radionuclide concentrations using the dehoog method
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3. TECHNICAL DESCRIPTION

The basic theoretical and mathematical models, the data flow, process flow, control flow and control logic are identical to those described in the User's Manual of TOUGH2 V1.11MEOS9NT V1.0 (Moridis et al., 1999). The basic structure modification is the introduction of modules to replace the older concept of COMMON blocks in older forms of FORTRAN (e.g., FORTRAN77). One of the first modules used by the code allows dynamic memory allocation, thus eliminating the need to re-dimension the code for different size problems.

3.1 THEORETICAL BASIS

TOUGH2 V1.11MEOS9NTV2.0 can simulate flow and transport of an arbitrary number n of nonvolatile tracers (solutes and/or colloids) in the subsurface. EOS9NT first solves the Richards equation, which describes saturated or unsaturated water flow in subsurface formations, and obtains the flow regime. The set of n linearly independent transport equations (corresponding to the n solutes/colloids) are then solved sequentially. The n tracer transport equations account for (a) advection, (b) molecular diffusion, (c) hydrodynamic dispersion (with full 3-D tensorial representation), (d) kinetic or equilibrium physical and chemical sorption (linear, Langmuir, Freundlich, or combined), (e) first-order linear chemical reaction, (e) radioactive decay, (f) colloid filtration (equilibrium, kinetic or combined), and (g) colloid assisted solute transport. A total of $n - 1$ daughter products of radioactive decay (or of a linear, first-order reaction chain) can be tracked.

The flow component in EOS9NT is based on the EOS9 module (Wu et al. 1996; Wu and Mishra 1998), in which a single equation is solved. This is the Richards (1931) equation, which describes the flow of water in the subsurface under saturated or unsaturated conditions under the following assumptions:

1. The water flow is isothermal
2. The concentration of the solutes or colloids is at tracer level, i.e., too low to have any measurable effect on the flow regime.
3. The pressure of the gaseous phase does not deviate significantly from the reference pressure of the system
4. There is no phase change.

These assumptions allow decoupling of the flow and transport equations. The Richards equation is first solved, followed by the sequential solution of the n independent tracer transport equations. If any combination of assumptions (1), (2), and (4) does not hold true, then the combination EOS3nT module (Moridis et al. 1999) must be used.

EOS9NT includes two types of Laplace transform formulations of the tracer equations, in addition to conventional timestepping. The Laplace transform is applicable to steady-state flow

fields and allows a practically unlimited time-step size and more accurate solution (as numerical diffusion is significantly reduced).

3.2 MATHEMATICAL MODEL

3.2.1 General Mass Balance Equations

Following Pruess (1987 [100684]; 1991 [100413]), mass balance considerations in a control volume dictates that

$$\frac{d}{dt} \int_{V_n} M_{\kappa} dV = \int_{\Gamma_n} \mathbf{F}_{\kappa} \cdot \mathbf{n} d\Gamma + \int_{V_n} q_{\kappa} dV \quad (\text{Eq. 3-1})$$

where

- V, V_n = volume, volume of subdomain n [L^3]
- M_{κ} = mass accumulation term of component (tracer) κ [ML^{-3}]
- Γ, Γ_n = surface area, surface area of subdomain n [L^2]
- \mathbf{F}_{κ} = Darcy flux vector of component κ [$ML^{-2}T^{-1}$]
- \mathbf{n} = inward unit normal vector [L^0]
- q_{κ} = source/sink term of tracer κ [$ML^{-3}T^{-1}$]
- t = time [T].

The conservation of mass for any subdomain n is given by Equation 3-1, which in space-discretized form assumes the form of the following ordinary differential equation:

$$\left(\frac{dM_{\kappa}}{dt} \right)_n = \frac{1}{V_n} \sum_m A_{nm} (F_{\kappa})_{nm} + (q_{\kappa})_n \quad (\text{Eq. 3-2})$$

where A_{nm} is the surface segment between elements n and m [L^2], $(F_{\kappa})_{nm}$ is the mass flux of tracer κ between elements n and m [$ML^{-2}T^{-1}$], and $(q_{\kappa})_n$ is the mass rate of the source/sink of tracer κ in element n [$ML^{-3}T^{-1}$]. Equation 3-2 is general, and applies to solutes and colloids.

3.2.2 Accumulation Terms

3.2.2.1 Equations of the Accumulation Terms

The accumulation term M of a tracer κ (solute or colloid) in a porous or fractured medium (PFM) is given by

$$M_{\kappa} = \begin{cases} M_{L,\kappa} + M_{Ag,\kappa} + \delta_R M_{R,\kappa} + \delta_c M_{Ac,\kappa} & \text{for solutes} \\ M_{L,\kappa} + M_{F,\kappa} + \delta_R M_{R,\kappa} & \text{for colloids} \end{cases}$$

$$M_{\kappa} = \begin{cases} M_{L,\kappa} + M_{Ag,\kappa} + \delta_c M_{Ac,\kappa} & \text{for solutes} \\ M_{L,\kappa} + M_{F,\kappa} & \text{for colloids} \end{cases} \quad (\text{Eq. 3-3})$$

where

$M_{L,\kappa}$ = the mass of tracer κ in the aqueous phase [ML^{-3}]

$M_{Ag,\kappa}$ = the mass of solute tracer κ adsorbed onto the PFM grains [ML^{-3}]

$M_{R,\kappa}$ = the reacted mass of tracer i (solute or colloidal) in the aqueous phase [ML^{-3}]

$M_{Ac,\kappa}$ = the mass of solute tracer κ adsorbed onto colloidal particles [ML^{-3}]

$M_{F,\kappa}$ = the mass of filtered colloidal tracer κ [ML^{-3}]

and the parameter

$$\delta_r = \begin{cases} 1 & \text{for reactive solutes or reactive "real" colloids} \\ 0 & \text{for solutes} \end{cases}$$

and

$$\delta_c = \begin{cases} 1 & \text{for "pseudocolloids"} \\ 0 & \text{for solutes} \end{cases} \quad (\text{Eq. 3-4})$$

The term "real" colloids refers to those generated from contaminants [Saltelli et al. 1984] when their concentrations exceed their solubility [van der Lee et al., 199], and their study focuses on their transport. Colloids from other sources (e.g. clay particles naturally occurring in the subsurface) are termed "pseudocolloids" [Ibaraki and Sudicky, 1995], and their study includes both colloid transport and sorption or contaminants onto them. EOS9NT allows the study of both types of colloids.

Omitting for simplicity the κ subscript, M_L is obtained from

$$M_L = \phi (S_w - S_r) \rho X + \phi S_r \rho X \quad (\text{Eq. 3-5})$$

where

X = the mass fraction of the tracer in the mobile fraction of the aqueous phase [M/M]

X = the mass fraction of the tracer in the immobile fraction of the aqueous phase [M/M]

S_w = the water saturation [L^3/L^3]

S_r = the immobile water saturation (can be set equal to the irreducible) [L^3/L^3]

ϕ = the porosity (matrix or fracture) [L^3/L^3]

ρ = the water density [ML^{-3}].

Equation 3-5 reflects the fact that solute concentrations are different in the mobile and immobile water fractions. Because water is very strongly bound (in electric double layers) to the PFM grain surface, Brownian motion is limited and solubility in the immobile water is lower than in the mobile water fraction. The importance of this boundary layer has been recognized by de

Marsily (1986 [100439], p. 234), who differentiates X and X , and Moridis (1999 [117241]), who used the mobile fraction of water in the analysis of diffusion experiments. Using the linear equilibrium relationship (Moridis 1999 [117241]),

$$X = K_i X \quad (\text{Eq. 3-6})$$

where K_i is a dimensionless mass transfer coefficient, for solutes $1 \geq K_i > 0$. Because of their double layers and their relatively large size (compared to solutes), colloids are expected to concentrate in the mobile water fraction and to be less abundant in the immobile water fraction. Thus, a good approximation of K_i for colloids would be $K_i < 1$, but we have not been able to find any good support in the literature.

Substitution into Equation 3-5 then leads to

$$M_L = \phi h \rho X, \quad \text{where } h = S_w - S_r + K_i S_r$$

3.2.3 Sorption Terms

Omitting again for simplicity the κ subscript, the mass of a solute sorbed onto the PFM grains and following a linear equilibrium isotherm is given by

$$M_{Ag} = (1 - \phi) \rho_s F \quad (\text{Eq. 3-8})$$

where

- ρ_s = the rock density [ML^{-3}];
- $F = F_p + F_c$, the total sorbed mass of solute per unit mass of the PFM, [M/M];
- F_p = the physically sorbed mass of solute per unit mass of the PFM [M/M];
- F_c = the chemically sorbed mass of solute per unit mass of the PFM [M/M];

3.2.3.1 Equilibrium Physical Sorption

Following the concepts of de Marsily (1986 [100439], p. 234) and considering that sorption onto the soil grains occurs as the dissolved species diffuses through the immobile water fraction (Moridis 1999 [117241]), the equilibrium physical sorption is described by the equation

$$F_p = \begin{cases} K_d \rho K_i X & \text{for linear equilibrium (LE) sorption,} \\ K_F (\rho K_i X)^\beta & \text{for Freundlich equilibrium (FE) sorption,} \\ \frac{K_1 \rho K_i X}{1 + K_2 \rho K_i X} & \text{for Langmuir equilibrium (LAE) sorption} \end{cases} \quad (\text{Eq. 3-9})$$

where $K_d [M^{-1}L^3]$, $K_F [M^{-\beta}L^{3\beta}]$, β , $K_1 [M^{-1}L^3]$, and $K_2 [M^{-1}L^3]$ are sorption parameters specific to each solute and rock type. Of particular interest is the parameter K_d , called the distribution coefficient, which is the constant slope of the linear equilibrium adsorption isotherm of a solute in relation to the medium.

3.2.3.2 Kinetic Physical Sorption

If a kinetic isotherm is followed, then sorption is described by equations given by

$$\frac{dF_p}{dt} = \begin{cases} k_\ell (K_d \rho K_i X - \delta_p F_p) & \text{for linear kinetic (LKP) sorption,} \\ k_F [K_F (\rho K_i X)^\beta - F_p] & \text{for Freundlich kinetic (FKP) sorption,} \\ k_L \left(\frac{K_1 \rho K_i X}{1 + K_2 \rho K_i X} - F_p \right) & \text{for Langmuir kinetic (LAKP) sorption,} \end{cases} \quad (\text{Eq. 3-10})$$

where

$$\delta_p = \begin{cases} 1 & \text{for linear kinetic physical (LKP) sorption;} \\ 0 & \text{for linear irreversible physical (LIP) sorption,} \end{cases} \quad (\text{Eq. 3-11})$$

and k_ℓ , k_F , and k_L are the kinetic constants for linear, Freundlich and Langmuir sorption, respectively [T^{-1}] (de Marsily (1986 [100439])). For $\delta_p=0$, the linear kinetic expression in Equation 3-9 can also be used to describe the chemical process of salt precipitation.

3.2.3.3 Kinetic Chemical Sorption

The first-order reversible chemical sorption is represented by the linear kinetic chemical (LKC) model

$$\frac{dF_c}{dt} = k_c^+ \rho K_i X - k_c^- F_c \quad (\text{Eq. 3-12})$$

where $k_c^+ [M^{-1}L^3T^{-1}]$ and $k_c^- [T^{-1}]$ are the forward and backward kinetic constants, respectively. Note that Equation 6-11 can be used in conjunction with the physical sorption equations to describe combined sorption (Cameron and Klute 1977 [117172]), e.g., physical and chemical sorption. Combined sorption accounts for the different rates at which a species is sorbed onto different PFM constituents. Thus, sorption onto organic components may be instantaneous (LE), while sorption onto mineral surfaces may be much slower and kinetically controlled (Cameron and Klute 1977 [117172]).

3.2.3.4 Chemical Reaction Terms

Assuming that reactions occur only in the liquid phase, the mass of reacted tracer (solute or colloid) is given by

$$M_R = \phi h \rho R \quad (\text{Eq. 3-13})$$

And R is obtained from the reaction kinetics. The kinetic equation of a chain of N_x first-order chemical reactions are given by (Cho, 1971)

$$\begin{aligned} \frac{\partial R_1}{\partial t} &= \kappa_1 \rho X_1, \\ \frac{\partial R_1}{\partial t} &= \kappa_2 \rho X_2 - \kappa_1 \rho X_1 \end{aligned} \quad (\text{Eq. 3-14})$$

$$\frac{\partial R_{N_x}}{\partial t} = \kappa_{N_x} \rho X_{N_x} - \kappa_{N_x-1} \rho X_{N_x-1}$$

Where κ_j ($j = 1, \dots, N_x$) is the chemical reaction rate constant and N_x is the number of chemical reactions in the chain. Implicit in equation (3-13) is the consideration of mass transfer through the immobile water fraction. Equation (3-13) and (3-14) apply to reactive solutes and reactive “true” colloids.

3.2.4 Colloid Filtration Terms

3.2.4.1 Equations of Colloid Filtration

Colloidal particles moving through porous media are subject to filtration, the mechanisms of which have been the subject of several investigations (e.g., Herzig et al. 1970 [117519]). The mass of filtered colloids is then given by

$$M_{F,\kappa} = \rho_{c,\kappa} \sigma_\kappa \quad (\text{Eq. 3-15})$$

where $\rho_{c,\kappa}$ is the density of the colloidal particles of colloid κ [ML^{-3}] and σ_κ is the filtered concentration of the colloid expressed as volume of colloids per volume of the porous medium.

When colloid deposition is a relatively fast process compared to the water velocity, it is possible to describe colloid filtration as a linear equilibrium process (James and Chrysikopoulos 1999 [109517]). Omitting the κ subscript, linear equilibrium filtration is then described by

$$\sigma = K_\sigma K_i \rho X \quad (\text{Eq. 3-16})$$

where K_σ is a distribution coefficient [$M^{-1}L^3$] and K_i is a dimensionless mass transfer coefficient.

Colloid filtration is more accurately described by a linear kinetic model (Çorapçıoğlu et al. 1987 [117300], pp. 269–342), which can take the following form:

$$\frac{d\sigma}{dt} = \kappa(K_\sigma K_i \rho X - \delta_p \sigma) = \kappa^+ X - \kappa^- \sigma \quad (\text{Eq. 3-17})$$

where κ [T^{-1}] is a kinetic coefficient, and κ^+ and κ^- [T^{-1}] are the kinetic forward and reverse colloid deposition rates (clogging and declogging coefficients), respectively, which are specific to each colloid and rock type. The term κ^- is commonly assumed to be zero (Bowen and Epstein 1979 [117219]), but there is insufficient evidence to support this. The parameter δ_p is analogous to that for sorption in Equations 3-10 and 3-11, and describes the reversibility of filtration.

From de Marsily (1986 [100439], p. 273) and Ibaraki and Sudicky (1995 [109297], p. 2,948), the following expression for the κ^+ coefficient can be derived:

$$\kappa^+ = \varepsilon f u G \quad (\text{Eq. 3-18})$$

where ε is the filter coefficient of the porous medium [L^{-1}], f is a velocity modification factor, u is the Darcy velocity [LT^{-1}], and G is a dynamic blocking function that describes the variation of the PFM porosity and specific surface with σ (James and Chrysikopoulos 1999 [109517]). The factor f ($1 \leq f \leq 1.5$) accounts for the velocity of the colloidal particle flow being larger than that of water (Ibaraki and Sudicky 1995 [109297], p. 2,948). This results from the relatively large size of the colloids, which tends to concentrate them in the middle of the pores where the water velocity is larger than the bulk average velocity. The factor f tends to increase with decreasing ionic strength, but cannot exceed 1.5 because colloids cannot move faster than the maximum water velocity, which occurs at the middle of the pores and is equal to 1.5 the average pore velocity (Ibaraki and Sudicky 1995 [109297], p. 2,948).

For deep filtration (i.e., in the case of very dilute colloidal suspensions), there is no interaction among the colloidal particles and no effects on the medium porosity and permeability, i.e., ϕ is constant, and $G=1$. Note that it is possible for EOS9NT to have combined filtration, in which two different types of filtration (e.g., equilibrium and kinetic, or two kinetic filtrations with different κ^+ and κ^-) occur simultaneously.

3.2.5 Colloid-Assisted Transport Terms

3.2.5.1 Equations of Colloid-Assisted Transport

The mass of a tracer κ sorbed onto pseudocolloids is described by

$$M_{Ac, \kappa} = \sum_{j=1}^{N_c} (\rho_j \sigma_j + \rho X_j) F_{\kappa, j} \quad (\text{Eq. 3-19})$$

where $F_{\kappa j}$ denotes the sorbed mass of solute κ per unit mass of the pseudocolloid j [M/M] and N_c is the total number of pseudocolloid species (Moridis et al. 1999 [123093]). The first term in the sum inside the parenthesis of Equation 3-17 describes the filtered (deposited) colloid concentration, and the second describes the concentration of the suspended colloids in the liquid phase. $F_{\kappa j}$ is computed from any combination of Equations (3-9) – (3-12), with the appropriate sorption parameters corresponding to each colloid. Note that Equation (3-19) applies to pseudocolloids only, as opposed to true colloids, onto which radionuclides are not considered to sorb.

3.2.6 Flux Terms

3.2.6.1 Equations of the Flux Terms

The flux term has contributions from advective, diffusive, and dispersive transport processes and is given by

$$\mathbf{F}_{\kappa} = \mathbf{F}_{\omega} X_{\kappa} - \rho \mathbf{D}_{\kappa} \nabla X_{\kappa} - \mathbf{F}_{s, \kappa} \quad (\text{Eq. 3-20})$$

where \mathbf{F}_{ω} is water flux term, $\mathbf{F}_{s, \kappa}$ is the flux due to surface diffusion, and \mathbf{D}_{κ} is the dispersion tensor of tracer κ , a second order symmetric tensor with a principal axis aligned with the Darcy flow vector. Omitting the κ subscript, \mathbf{D} is described by the equations

$$\mathbf{D} = D^T \mathbf{I} + \frac{D^L - D^T}{u^2} \mathbf{u} \mathbf{u}, \quad (\text{Eq. 3-21})$$

$$D^L = \phi S_w \tau D_0 + \alpha_L u \quad (\text{Eq. 3-22})$$

$$D^T = \phi S_w \tau D_0 + \alpha_T u \quad (\text{Eq. 3-23})$$

where

\mathbf{I} = the unit vector

τ = the tortuosity coefficient of the pore paths [L/L]

D_0 = the molecular diffusion coefficient of tracer i in water [$L^2 T^{-1}$]

α_L, α_T = longitudinal and transverse dispersivities, respectively [L]

\mathbf{u} = the Darcy velocity vector [LT^{-1}]

Equation (3-20) accounts for surface diffusion, which can be responsible for significant transport in strongly sorbing media (Moridis 1999 [117241]; Cook 1989 [117314]). The surface diffusion flux is given by Jahnke and Radke (1987 [117398]) as

$$\mathbf{F}_s = (1 - \phi) \rho_s \tau_s D_s \nabla F_p, \quad (\text{Eq. 3-24})$$

where τ_s is the tortuosity coefficient of the surface path [L^0], D_s is the surface diffusion coefficient [L^2T^{-1}], and F_p is the physical diffusion computed from equations (3-9) or (3-10).

There is theoretical justification for the relationship $\tau_s = \frac{2}{3} \tau$ (Cook 1989 [117314], p. 10).

3.2.6.2 The dispenser tensor.

In the treatment of the general 3-D dispersion tensor, EOS9NT follows closely the approach of the radionuclide transport module T2R3D (Wu et al., 1996; Wu and Mishra, 1998) for TOUGH2. Velocities are averaged by using the projected area weighting method, in which a velocity component u_i ($j=x,y,z$) of the vector u is determined by vectorial summation of the components of all local connection vectors in the same direction, weighted by the projected area in that direction. This approach allows the solution of the transport problem in irregularly-shaped grids, in which the velocities normal to the interface areas are not aligned with the principal axes.

3.2.6.3 Application to Colloid Fluxes.

Equations (3-17) through (3-20) apply to solutes, but need the following modifications to render them suitable to colloidal transport. More specifically:

1. $F_s = 0$ because surface diffusion does not occur in colloids.
2. The flux F_s and the Darcy velocities u are multiplied by the factor f (see Section 3.2.4.1).
3. The dispersivities α_L and α_T are generally different from those for solutes Ibaraki and Sudicky (1995) and may be a function of the colloidal particle size.
4. The term D_0 is the colloidal diffusion coefficient in water [L^2T^{-1}] and is described by the Stokes-Einstein equation, according to Bird et al. (1960, p. 514), as

$$D_0 = \frac{kT}{3\pi\mu_w d_p}, \quad (\text{Eq. 3-25})$$

where k is the Boltzmann constant ($1.38 \times 10^{-23} JK^{-1}$ in SI units), T is the absolute water temperature [K], μ_w is the dynamic viscosity of water [$ML^{-1}T^{-1}$], and d_p is the colloid diameter [L].

5. The fluxes in Equation (3-20) are multiplied by the colloid accessibility factors f_c ($0 \leq f_c \leq 1$) at the interface of different media. The f_c factor describes the portion of the colloidal concentration in a medium that is allowed to enter an adjacent medium of different characteristics, and quantifies pore size exclusion (straining).

3.2.7 Radioactive Decay

3.2.7.1 Equations of Radioactive Decay

When a tracer κ undergoes radioactive decay, the rate of mass change is described by the first-order decay law

$$\frac{dM_{\kappa}}{dt} = -\lambda_{\kappa}M_{\kappa}, \quad \text{where} \quad \lambda_{\kappa} = \frac{\ln 2}{(T_{1/2})_{\kappa}} \quad (\text{Eq. 3-26})$$

and $(T_{1/2})_{\kappa}$ is the half life of tracer κ . Substitution of Equations 3-20 and 3-26 into Equation 3-2 yields (Moridis et al. 1999 [123093] Eq. 32)

$$\left(\frac{dM_{\kappa}}{dt} \right)_n + \lambda_{\kappa}(M_{\kappa})_n = \frac{1}{V_n} \sum_m A_{nm} [F_{nm}X_{\kappa} - \rho D_{\kappa} \nabla X_{\kappa} - F_{s,\kappa}] + (q_{\kappa})_n \quad (\text{Eq. 3-27})$$

3.2.7.2 Implications for Transport in the UZ

The decay of radioactive substance is completely predictable and well documented. Thus, the decay of radioactive substances in Unsaturated Zone (UZ) simulations can be computed very reliably.

3.2.8 Daughter Products of Radioactive Decay

3.2.8.1 Transport Equations of Daughters

If a radioactive tracer κ is a daughter product of the decay of tracer j , then the mass accumulation terms are adjusted (de Marsily 1986 [100439], pp. 265–266) to yield the equation of transport of the daughter products as

$$\begin{aligned} & \left(\frac{dM_{\kappa}}{dt} \right)_n + \lambda_{\kappa}(M_{\kappa})_n - \lambda_j m_r (M_j)_n \\ & = \frac{1}{V_n} \sum_m A_{nm} [F_{nm}X_{\kappa} - \rho D_i \nabla X_{\kappa} - F_{s,\kappa} + (q_{\kappa})_n \end{aligned} \quad (\text{Eq. 3-28})$$

where $m_r = W_{\kappa}/W_j$, and W_{κ} and W_j are the molecular weights of the daughter and parent species. Equation (3-28) applies to radioactive solutes or radioactive true colloids.

For daughters following an isotherm other than LE, Equations (3-10) and (3-12) need to account for the generation of daughter mass from the decay of the sorbed parent, and become

$$\frac{\partial F_{\kappa}}{\partial t} + \lambda_{\kappa}F_{\kappa} - \lambda_{\kappa-1}m_r\zeta_{\kappa}F_{\kappa-1} = k_A\rho X_{\kappa} - k_B(F_{\kappa} + m_r\zeta_{\kappa}F_{\kappa-1}) \quad (\text{Eq. 3-29})$$

where $F_{\kappa-1}$ is the sorbed mass of the parent,

$$k_A = \begin{cases} k_\ell K_d K_i & \text{for LKP/LIP sorption} \\ k_c^+ K_i & \text{for LKC sorption} \end{cases} \quad k_B = \begin{cases} k_p \delta_p & \text{for LKP/LIP sorption,} \\ k_c^- & \text{for LKC sorption,} \end{cases} \quad (\text{Eq. 3-30})$$

and ζ_κ is the fraction of the mass of the decayed sorbed parent that remains sorbed as a daughter ($0 \leq \zeta_\kappa \leq 1$). The term ζ_κ is introduced to account for the different sorption behavior of parents and daughters, and the fact that daughters can be ejected from grain surfaces due to recoil (e.g., the ejection of ^{234}Th from grain surfaces during the alpha decay of ^{238}U) (Faure 1977 [122805], pp. 288–289). The right-hand side of Equation 3-29 is analogous and can be modified for Freundlich and Langmuir kinetic model (see Equation 3-10).

3.3 CONTROL LOGIC

EOS9NT V2.0 is controlled internally by variables in the input file. There are no user interface interactively controlling input and output parameters during execution. User is supposed to provide input parameters as an input file. Input and output file names should be provided when the software is executed.

3.4 DATA STRUCTURES

For general description of input data needed for the code, see Attachment A. Output data generated by the code is described in Attachment B.

3.5 CONTROL FLOW

There are no user interface controls during execution. See Attachment C for flow chart.

3.6 DATA FLOW

For the data flow see flow chart in Attachment C.

4. INPUT/OUTPUT

4.1 INPUT RANGES

Inputs to EOS9NT V2.0 include both the standard inputs required by the previous version (TOUGH2 V1.11MEOS9NT V1.0) (Pruess et al., 1999). The inputs include (a) parameters to describe the hydraulic properties of the rocks, (b) the discretized simulation domain, as described by the grid and its geometric properties, (c) the transport parameters (related to diffusion and sorption) of the various tracers in the various rocks, (d) the sources and sinks, (e) the initial conditions (pressure, temperature, tracer concentration), and (f) basic parameters that control the simulation. The options and ranges of the basic simulation parameters are controlled internally, and error messages are printed if improper values are selected. The concentration input is in terms of mass fraction, thus its range is between 0 and 1.

A new set of inputs that are needed to implement the capabilities of the new version includes dynamic memory allocation, 8-character cell naming, and new colloid transport features. See Attachment A for description of the EOS9NT V2.0 input specifications.

4.2 OUTPUT RANGES

The concentration output is in terms of mass fraction, thus its range is between 0 and 1. Output data generated by the code is listed and described in Attachment B.

5. TEST PLAN

The performance of EOS9NT is to be tested against a set of 1-D and 2-D problems with known analytical solutions. When no analytical solutions are available (e.g., in the case of solute transport into an unsaturated soil), the EOS9NT results are to be compared to those from other numerical codes. EOS9NT results are to be obtained for all three possible treatments of time, i.e., for conventional time-stepping (hereafter referred to as the T-solution) and, when possible, for the two Stehfest and De Hoog Laplace space formulations (hereafter referred to as the S and H solutions, respectively).

The testing approach involves the following steps:

- (a) Regression analysis (testing against results, where applicable, of the qualified TOUGH2 V1.11MEOS9NT V1.0, Moridis, 2000) and comparison to validated analytical and/or numerical solutions.
- (b) Testing to demonstrate adequacy of the Requirements, as described in the Requirements Document [10065-RD-1.11MEOS9NTV2.0-01]

5.1 ACCEPTANCE CRITERIA

The quantitative acceptance criteria for all cases are for the EOS9NT results to be within 5% of the analytical or other numerical code comparison value(s). The qualitative acceptance criteria are that the execution terminates without error.

5.2 TEST CASES

Test Cases are identified by number (TC ID) with reference to the related design components (DC ID)

Execution Instruction—Refer to the User Information Document, where the actual execution instructions shall be provided.

TC ID	DC ID	Requirement ID	Test Case
TC-01	DC-01 DC-02 DC-03 DC-04 DC-05 DC-06	FR-01 FR-02 FR-03 FR-04 FR-05 FR-06 FR-07 DCR-01 AR-01 ER-01 ER-02 ER-03	Transport of a non-decaying, non-sorbing (conservative) tracer through porous media Step #1: Description: This test simulates the transport of a non-decaying, non-sorbing (conservative) tracer through porous media. We follow the procedure described above. We use the input file "Test_1b_T" and the corresponding initial condition file "INCON_b". After moving these two files to the code folder/directory, rename the "INCON_b" file "INCON", and run the simulation.

			<p>There is no fixed memory allocation (dimensioning) in EOS9NT V2.0. Thus, by being able to run this (and any other test problems), we validate the ability of EOS9NT V2.0 to employ dynamic memory allocation.</p> <p>Comparison of the output to that from the qualified TOUGH2 V1.11MEOSE9NT V1.0 code, and to the analytical solutions verifies the code through (a) the regression analysis, and (b) the accuracy of predictions of conservative tracer transport (vis-à-vis the analytical results).</p> <p>Step #2: Description: The test is repeated by employing the same INCON file and different time treatment options (i.e., the input files with the “_S” and “_H” suffixes).</p> <p>Comparison of the output to (a) that from the qualified TOUGH2 V1.11MEOSE9NT V1.0 code, (b) the results in Step #1, and (c) to the analytical solutions of Bear (1979) verifies the code through (1) the regression analysis, and (2) the accuracy of predictions of conservative tracer transport (vis-à-vis the analytical results).</p>
TC-02	DC-01 DC-02 DC-03 DC-04 DC-05 DC-06	FR-01 FR-02 FR-03 FR-04 FR-05 FR-06 FR-07 DCR-01 AR-01 ER-01 ER-02 ER-03	<p>Transport of a decaying, sorbing radioactive 3-member chain through porous media</p> <p>Step #1: Description: This test simulates the transport of a decaying, sorbing radioactive 3-member chain through porous media. We follow the procedure described above. We use the input file “Test_2_T” and the corresponding initial condition file “INCON”.</p> <p>There is no fixed memory allocation (dimensioning) in EOS9NT V2.0. Thus, by being able to run this (and any other test problems), we validate the ability of EOS9NT V2.0 to employ dynamic memory allocation.</p> <p>Comparison of the output to that from the qualified TOUGH2 V1.11MEOSE9NT V1.0 code, and to the analytical solutions verifies the code through (a) the regression analysis, and (b) the accuracy of predictions of transport of radioactive chains (vis-à-vis the analytical results).</p> <p>Step #2: Description: The test is repeated by employing the same</p>

			<p>INCON file and different time treatment options (i.e., the input files with the “_S” and “_H” suffixes).</p> <p>Comparison of the output to (a) that from the qualified EOS9NT V1.0 code, (b) the results in Step #1, and (c) to the analytical solutions of Harada et al. (1980) verifies the code through (1) the regression analysis, and (2) the accuracy of predictions of transport of radioactive chains (vis-à-vis the analytical results).</p>
TC-03	DC-01 DC-02 DC-03 DC-04 DC-05 DC-06	FR-01 FR-02 FR-03 FR-04 FR-05 FR-06 FR-07 DCR-01 AR-01 ER-01 ER-02 ER-03	<p>Transport of a radioactive species in a fracture-matrix system</p> <p>Step #1: Description: This test simulates the transport of a radioactive species in a fracture-matrix system. We follow the procedure described above. We use the input file “Test_3_H” and the corresponding initial condition file “INCON”.</p> <p>There is no fixed memory allocation (dimensioning) in EOS9NT V2.0. Thus, by being able to run this (and any other test problems), we validate the ability of EOS9NT V2.0 to employ dynamic memory allocation.</p> <p>Step #2: Description: The test is repeated by employing the same INCON file and different time treatment options (i.e., the input files with the “_S” and “_T” suffixes).</p> <p>Comparison of the output to that from the qualified TOUGH2 V1.11mEOSE9nT V1.0 code, and to the analytical solutions verifies the code through (a) the regression analysis, and (b) the accuracy of predictions of radioactive transport in fracture-matrix systems.</p>
TC-04	DC-01 DC-02 DC-03 DC-04 DC-05 DC-06	FR-01 FR-02 FR-03 FR-04 FR-05 FR-06 FR-07 DCR-01 AR-01 ER-01 ER-02	<p>Simultaneous water flow and tracer transport through an unsaturated medium</p> <p>Step #1: Description: This test simulates the simultaneous water flow and tracer transport through an unsaturated medium. We follow the procedure described above. We use the input file “Test_4” and the corresponding initial condition file “INCON”.</p> <p>There is no fixed memory allocation (dimensioning) in</p>

		ER-03	<p>EOS9NT V2.0. Thus, by being able to run this (and any other test problems), we validate the ability of EOS9NT V2.0 to employ dynamic memory allocation.</p> <p>There is an analytical solution to the problem of water saturation evolution (Philip, 1995), but no analytical solutions for the corresponding transport problems. Comparison of the output to that from the analytical saturation solution, to that from the qualified TOUGH2 V1.11MEOSE9NT V1.0 code, and to that from the EOS7R code (Oldenburg and Pruess, 1995) verifies the code through (a) the regression analysis, and (b) consistency of predictions.</p>
TC-05	DC-01 DC-02 DC-03 DC-04 DC-05 DC-06	FR-01 FR-02 FR-03 FR-04 FR-05 FR-06 FR-07 DCR-01 AR-01 ER-01 ER-02 ER-03	<p>Simultaneous water flow and tracer transport through an unsaturated medium (8-character element names)</p> <p>Step #1: Description: This test simulates the simultaneous water flow and tracer transport through an unsaturated medium. We follow the procedure described above. We use the input file "Test_5_H" and the corresponding velocity file "VELOC".</p> <p>There is no fixed memory allocation (dimensioning) in EOS9NT V2.0. Thus, by being able to run this (and any other test problems), we validate the ability of EOS9NT V2.0 to employ dynamic memory allocation. Ability of the code to run this problem fulfills the requirement that EOS9NT V2.0 be able to handle 8-character element names.</p> <p>Step #2: Description: The test is repeated by employing different time treatment options (i.e., the input file with the "_S" suffix).</p> <p>There is no analytical solution to this problem. Comparison of the output to that from the qualified T2R3D code (Wu et al., 1996) verifies the code through the agreement and consistency of the solutions. The acceptance criterion in this case is agreement within 5% of the breakthrough curves computed from the results of the EOS9NT V2.0 solution and of the T2R3D solutions.</p>
TC-06	DC-01 DC-02 DC-03 DC-04	FR-01 FR-02 FR-03 FR-04	<p>Transport of colloids (e.g., clays), onto which radioactive species are sorbed reversibly and irreversibly</p> <p>Step #1:</p>

	DC-05 DC-06	FR-05 FR-06 FR-07 DCR-01 AR-01 ER-01 ER-02 ER-03	<p>Description: This test simulates the transport of colloids (e.g., clays), onto which radioactive species are sorbed reversibly and irreversibly. We follow the procedure described above. We use the input file "Test_6" and the corresponding velocity file "VELOC".</p> <p>There is no fixed memory allocation (dimensioning) in EOS9NT V2.0. Thus, by being able to run this (and any other test problems), we validate the ability of EOS9NT V2.0 to employ dynamic memory allocation.</p> <p>Comparison of the output to the analytical solution of Dieulin (de Marsily, 1982) verifies the ability of the code to predict colloid transport. Comparison of the relative mass ratios of the irreversibly sorbed radionuclides to analytical predictions verifies the ability of the code to predict transport of radioactive species through irreversible sorption onto pseudocolloids.</p>
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The expected outputs of validation tests are available from User Information Document for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-UID-1.11MEOS9NTV2.0-01).

6. REFERENCES/ATTACHMENTS

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IT-PRO-0012, Rev.0. Qualification of Software. DOC.20060228.0007

IT-PRO-0013, Rev.0. Software Independent Verification and Validation. DOC.20060228.006

Software Configuration Control Request for TOUGH2 V1.11MEOS9NT V2.0. (Software Tracking Number: 10065-1.11MEOS9NTV2.0-01)

6.2 ATTACHMENTS

Attachment A: Input Data Requirements and Specifications

Attachment B: Output Data

Attachment C: Flow Chart

ATTACHMENT A. INPUT DATA REQUIREMENTS AND SPECIFICATIONS

A.1. DATA BLOCK ALLOC

This is a new data block that sets the parameters for the dynamic memory allocation implemented in EOS9NT V2.0. Because there is no *a priori* array dimensioning, this block must always be placed at the beginning of the input data file. Failure to do so prevents memory allocation and causes fatal errors in the attempt to run EOS9NT V2.0. The data block consists of several cards, which are assemblage of parameters to be read by a line to the EOS9NT V2.0.

A.1.1. Card ALLOC.1

This card must always include the following character string:

```
TOUGH2/EOS9NT MEMORY ALLOCATION
```

starting at the leftmost field location of the card. If this string is missing or is altered, a warning message is printed, and the simulation is aborted.

A.1.2. Card ALLOC.2

This card includes the following parameters:

```
MNEL, MNCON, No_CEN, FLG con
```

that are read according to

```
FORMAT ( 2 ( I10 ), I2, 2X, A6 )
```

These parameters are as follows:

MNEL	This parameter is standard to all members of the TOUGH2 family of codes [Pruess, 1987;1991], and represents the maximum expected number of elements in the grid.
MNCON	This parameter is standard to all members of the TOUGH2 family of codes, and represents the maximum expected number of connections in the grid.
No_CEN	The number of characters of the element names in the grid. There are two possible values of No_CEN. When No_CEN=5, then 5-character element names (the standard in TOUGH2) are used. When No_CEN=8, then 8-character element names are used, thus enabling simulations of extremely large grids. Note that, for No_CEN≠8, No_CEN is internally reset to the standard value of 5.
FLG_con	If the flag FLG_con='ACTIVE', EOS9NT checks the CONNE data block [Pruess, 1987;1991] for connections between inactive elements, prints a new CONNE block involving only active connections (i.e.,

connections involving at least one active element), and stops. This facility allows the reduction of the MNCON parameter in input files involving a very large number of inactive elements. By using only active connections, the memory requirements are reduced, and thus larger problems become tractable on the same computing platform.

A.1.3. Card ALLOC.3

This card includes the parameters MNOGN, MG TAB that are read according to the format in Section A.1.2. MNOGN and MG TAB are standard to all members of the TOUGH2 family of codes [Pruess, 1987;1991]. They represent the maximum expected number of sources and sinks, and the total number of points in tabular generation data.

A.1.4. Card ALLOC.4

This card includes the parameter NROKMX that is read according to the format in Section A.1.2. NROKMX represents the maximum expected number of rocks (i.e., media and/or formations with different hydraulic properties) in the EOS9NT simulation.

A.1.5. Card ALLOC.5

This card includes the parameter NTRCMX that is read according to the format in Section A.1.2. NTRCMX is the maximum expected number of tracers to be simulated simultaneously in each EOS9NT run.

A.2. DATA BLOCK ROCKS

A.2.1. Card ROCKS.1

If the parameter POR (i.e., the rock porosity) ≥ 2 , EOS9NT automatically sets ALPHAL=ALPHAT=0.0 in ROCKS.1.1 (see Section A.1.2). Moreover, it resets the tortuosity TORT=0.0 in card ROCKS.1.1. This allows the use of *atmospheric* gridblocks and alleviates the non-physical behavior of tracers diffusing into these gridblocks.

A.2.2. Card ROCKS.1.1

Card ROCKS.1.1 reads the following:

COM, EXPAN, CDRY, TORT, GK, SWIR, PORDIA, PHIF, PORD_SG
according to the format

FORMAT(9E10.4)

The parameters COM, EXPAN, CDRY, TORT, GK remain as previously described in TOUGH2 [Pruess, 1987;1991]. The other parameters are as follows.

SWIR	The immobile water saturation S_r . It is internally reset to 0.0 if SWIR > 1 or SWIR < 0
PORDIA	If the corresponding rock type describes a porous rock, PORDIA is mean pore diameter (m). If the rock type reflects the properties of a fracture,

PORDIA is the fracture aperture (m). This parameter is important in colloid transport, and the code will cease the simulation and print an error message if PORDIA= 0 and any colloid is among the simulated tracers. If $\text{PORDIA} \leq 0$, the pore sizes of the rock are assumed to be lognormally distributed, and $\text{ABS}(\text{PORDIA})$ is the mean of the $\ln(d_c)$ distribution.

PHIF The bulk fracture porosity of a fracture, defined as the ratio of the fracture pore volume to the bulk volume of the rock. This parameter is needed in dual permeability simulations of fractured rocks, and is needed to accurately compute diffusive and dispersive fluxes. For unfractured rocks, PHIF is not needed, and is reset internally to the rock porosity POR.

PORD_SG The standard deviation of the lognormally distributed $\ln(d_c)$. This parameter is only considered if $\text{PORDIA} \leq 0$. Otherwise, it is reset internally to zero. If $\text{PORDIA} \leq 0$ and $\text{PORD_SG} > 0$, then EOS9NT will compute internally the colloid accessibility factor f_c .

The card ROCKS.1.1 is necessary in EOS9NT. Even if $\text{NAD} = 0$ in ROCKS.1 ($\text{NAD} = 0$ indicates that no additional rock-related data lines are to be read, see Preuss et al. 1999), the code resets it internally to 1, and attempts to read the data values. For $\text{NAD} \geq 1$, there is no change. If the fields for ALPHAL and ALPHAT are left blank, zero values are assigned. The user is cautioned that the tortuosity TORT in card ROCKS.1.1 (i.e., the τ parameter) is important in the simulation of tracer transport, and that representative values should be used especially under diffusion-dominated regimes. Leaving the TORT field blank sets $\text{TORT} = 0.0$, and eliminates molecular diffusion in the simulation. The tortuosity of the surface diffusion paths τ_s is computed internally as $\tau_s = \tau$.

A.2.3. Domain REFCO

EOS9NT allows providing reference conditions through the use of a fictitious domain (rock) named REFCO. If a REFCO domain is present in rocks, then:

- (a) If $\text{DROK} \neq 0.0$, the reference gas pressure $P_g = \text{DROK}$.
- (b) If $\text{POR} \neq 0.0$, the reference temperature $T = \text{POR}$.
- (c) If $\text{PER}(1) \neq 0.0$, the reference water density $\rho = \text{PER}(1)$.
- (d) If $\text{PER}(2) \neq 0.0$, the reference water viscosity $\mu = \text{PER}(2)$.
- (e) If $\text{PER}(3) \neq 0.0$, the reference water compressibility $b_w = \text{PER}(3)$.
- (f) If $\text{CWET} \neq 0.0$, the reference elevation for gravity-capillary equilibrium $z = \text{CWET}$.
When $\text{CWET} \geq 10^5$ in domain REFCO, then gravity equilibration is performed using the water table elevation read as part of the ELEME data block.
- (g) If $\text{SPHT} \neq 0.0$, it specifies an optional index number of irreducible water saturation; this will cause water saturation to be specified at the irreducible level for strong capillary pressures.

If no REFCO domain is present, then the default initial conditions are: $P_g = 1.0103 \times 10^5$ Pa and $T = 15^\circ\text{C}$.

A.2.4. Domain SEED

When a domain SEED is present, modifiers (multipliers) shall be applied to the permeabilities k , and scaling shall be applied to the capillary pressures P_c . Denoting the permeability modifier with k_m , the modified permeability k^* becomes

$$k^* = k_m k ;$$

and the scaled capillary pressure P_c^* is to be given by

$$P_c^* = P_c / \sqrt{k_m}$$

The following options are available:

- (a) When DROK=POR=0.0 in domain SEED, the parameters PMX read as part of the ELEME data block will be used as modifiers (see discussion in Section A.4). However, when a file RANDOM is present, 10,000 PMX data will be read from it according to FORMAT(10(1X,E12.6)), overwriting the data in the ELEM data block.
- (b) When DROK≠0 random numbers will be generated internally with DROK as seed. A linear permeability modification will be made.
- (c) When DROK=0 and POR≠0, random numbers will be generated internally with POR as seed. A logarithmic permeability modification will be made.

In domain SEED, PER(1) is an optional scale factor. Random numbers will be generated in the interval (0, PER(1)). If w is a random number ($0 \leq w \leq 1$), the permeability modifiers k_m are:

- (a) $k_m = \text{PMX}$, when PMX are externally supplied
 - (b) $k_m = \text{PER}(1) * w$, when DROK≠0 (linear scaling)
 - (c) $k_m = \exp(-\text{PER}(1) * w)$, when DROK=0.0 and POR≠0 (logarithmic scaling)
- PER(2) is an optional shift: for PER(2) ≠ 0, the permeability modifiers used are $k_m = k_m - \text{PER}(2)$.

A.3. DATA BLOCK PARAM

A.3.1. Card PARAM.1

In EOS9NT, the computational parameters read in PARAM.1 are:

NOITE, KDATA, MCYC, MSEC, MCYPR, (MOP(I), I=1, 24),
DIFF0, TEXP, BE, ITRACR

and the format is

FORMAT(2I2, 3I4, 24I1, 3E10.4, I2)

All the parameters in PARAM.1 are as defined in [Pruess, 1987]. The new parameter ITRACR= n , i.e., the number of tracers under consideration. If ITRACR(≠0) differs from NTRACR in the data block TRACR in Section A.5, a warning of the discrepancy is printed and the simulation is aborted.

In EOS9NT V2.0 simulations, the parameter MOP(22) can be used to create ASCII data files ready for plotting, while the parameters MOP(23) and MOP(24) are important because their use can significantly reduce execution times.

A.3.1.1. The MOP (22) parameter.

If MOP (22) = 8 or 9, then EOS9NT V2.0 creates the following output files:

- (a) Plot_coord, in which the (x, y, z) coordinates of all the active elements are listed.
- (b) Plot_PSdat, which lists the pressure, saturation, capillary pressure, relative permeability, and intrinsic permeability of all the active elements in the indicated order.
- (c) *n* files named Plot_name, where 'name' is the name of each of the *n* tracers (the input parameter TRACER) that are simulated. The data listed in the Plot_name are
 - Relative mass fraction, mass fraction, primary sorption or infiltration, secondary sorption or infiltration (needed only in case of combined filtration, see Section 3.2.3.3), total sorption or infiltration – if the tracer is a colloid or a solute not involved in sorption onto colloids
 - Relative mass fraction, mass fraction, primary sorption, sorption onto mobile colloids, sorption onto immobile colloids (attached on the porous media) – if the tracer is a solute sorbing reversibly onto colloids (TRTYPE = SC).
 - Tracer mass ratio, mass fraction, primary sorption, sorption onto mobile colloids, sorption onto immobile colloids attached on the porous media through primary infiltration), sorption onto immobile colloids attached on the porous media through secondary infiltration – if the tracer is a solute sorbing irreversibly onto colloids (TRTYPE = SI).

These data can be read according to

```
FORMAT(6(1pe15.8,1x))
```

that is common to all files.

For the specific case of MOP (22) = 9, EOS9NT V2.0 computes and prints the cumulative fluxes across the outer boundaries of the systems. These are designated as occurring at the connections where one of the following scenarios holds true:

- (a) One of the connection elements is active and the other is inactive, with the first two characters of the inactive element's name being 'TP' (designating a top boundary) or 'BT' (indicating a bottom boundary).
- (b) One of the connection elements is active and the other is inactive, with the rock type of the inactive element having the name 'topbd' (designating a top boundary) or 'botbd' (indicating a bottom boundary).

A.3.1.2. The MOP (23) parameter.

If MOP (23) = 9 and the file UNVEC exists, then EOS9NT V2.0 does not compute the unit vectors normal to the gridblock interfaces, but instead reads this information, as well as information on the indices of the neighbors to each element involved in the connections. If the UNVEC file does not exist or MOP (23) ≠ 9, EOS9NT V2.0 creates the UNVEC file. Because the parameters in UNVEC are not easy to determine, this file must always be created by an EOS9NT V2.0 run. Note that the existence of the UNVEC file can drastically reduce execution times. In our experience from 3-D simulations involving grids of 100,000 gridblocks, this option can reduce execution times by about 65%. If the same grid is used for more than one simulations, the user is strongly urged to use this option. It is important, however, to ensure that MOP (23) ≠ 9 and/or no UNVEC file be present when the first simulation is attempted. Failure to do so can lead to serious

problems if the domain geometry implicit in UNVEC is in conflict with the one in the input file.

A.3.1.3. The MOP(24) parameter.

If $MOP(24) = 9$ and the file VELOC exists, then EOS9NT V2.0 does not solve the equations, but instead reads from VELOC the water flux, pore velocity, Darcy velocity, interface area, and upstream weighting factor at each connection. As in the case of $MOP(23)$, if the VELOC file does not exist or $MOP(23) \neq 9$, EOS9NT V2.0 creates the VELOC file. The user is strongly advised against attempting to develop this file, which should always be created by an EOS9NT V2.0 run. In conjunction with an UNVEC file, the presence of VELOC reduces execution times. If the same steady-state flow field is used for more than one simulations, the user is strongly urged to use this option. It is important, however, to ensure that $MOP(24) = 9$ and/or no VELOC file be present when (a) the first simulation is attempted and/or (b) the flow field is not time-invariant. Failure to do so can lead to serious problems if the domain geometry and/or the flow field in VELOC is in conflict with the ones in the input file.

A.3.2. Card PARAM.4

This card holds the primary variable $DEP(1)$ which is used as default initial conditions for all elements not specified in the data block INCON if the option START is selected. In EOS9NT, the card PARAM. 4 may hold one of the following:

- (a) The water pressure P [Pa] : $DEP(1) \geq 1$.
- (b) The water saturation: $0 \leq DEP(1) < 1$.
- (c) The capillary pressure: $DEP(1) < 0$.

Initialization of EOS9NT is possible using any of these three options. Additionally, initialization is possible from gravity-capillary pressure equilibrium based on elevation from the water table (an input). This last option is discussed in Sections A.2.3 and A.4.1.

A.3.3. Cards PARAM.4.1, PARAM.4.2, PARAM.4.3

These cards are mandatory if $ITRACR \neq 0$, in which case they hold (a) the default initial mass fractions X_i of the ITRACR tracers in the water, (b) the initial primary component of the sorbed or filtered mass (in kg of tracer per unit volume), and (c) the initial secondary component of the sorbed or filtered mass for combined sorption (in kg of tracer per unit volume), respectively, i.e.,

$$\begin{aligned} TMASSF(I), \quad I=1, \dots, ITRACR \\ XSOFIL(I), \quad I=1, \dots, ITRACR \\ XSOFI2(I), \quad I=1, \dots, ITRACR \end{aligned}$$

according to the format

$$FORMAT(4E20.13)$$

If colloid-assisted solute transport involving reversible sorption is studied ($TRTYPE = 'SC'$), then only primary sorption of the solute onto the porous medium can be considered. In this case, XSOFI2 represents the solute sorbed onto the sum of mobile and immobile (filtered) colloids, expressed as kg of solute per unit bulk volume). Note that all these card(s) (i.e., PARAM.4.1 to PARAM.4.3) are mandatory, regardless of whether sorption (primary and/or secondary) is

considered in the simulation.

A.4. DATA BLOCK ELEME

A.4.1. Card ELEME.1

In EOS9NT V2.0, the element information in ELEME. 1 can use the output of the MESHMAKER facility (module MESHM), but includes some additional information. More specifically, the following information is provided in ELEME. 1:

```
ELEM, MA1, MA2, VOLX, PMX, ZREF, XX, YY, ZZ
```

and the format for 5-character element names is

```
FORMAT (A5, 10X, A3, A2, 6 (E10.4))
```

or, for 8-character element names (see Section A.9.4),

```
FORMAT (A8, 7X, A3, A2, 6 (E10.4))
```

These parameters are defined as follows:

ELEM	The element name.
MA1, MA2	A five character material identifier corresponding to one of the domains (rocks) in data block ROCKS. If the first 3 characters are blank, the last two characters must be numbers, in which case they indicate the sequence number of the domain as entered in ROCKS.
VOLX	Element volume (m^3). If the second character in the element name is '*' (i.e., ELEME(2:2) = '*') or $VOLX > 10^{20} m^3$, the element is considered invariable (boundary), and is not considered in mass balance computations.
PMX	Permeability modifier (see Section A.2.4) for statistical heterogeneity applications.
ZREF	Reference watertable elevation for gravity-capillarity equilibration (m). It is invoked when the ZREF parameter in the REFCO domain (data block ROCKS) is $\geq 10^5$. Areal-ly-variable watertable elevations can thus be entered.
XX	x-coordinate of the gridblock center, with respect to a global coordinate system (m).
YY	y-coordinate of the gridblock center, with respect to a global coordinate system (m).
ZZ	z-coordinate of the gridblock center, with respect to a global coordinate system (m).

The PMX and ZREF fields may be blank. However, care must be taken to provide accurate information in the XX, YY and ZZ fields. This information is needed to determine the unit vectors at the centers of the two elements across each connection, which are used to determine the dispersion tensor. Inaccurate coordinate information will lead to erroneous results.

To maintain seamless compatibility with data files used in iTOUGH2 *Finsterle* [2002] simulations of flow fractured media, PMX can be negative (denoting fracture elements) and positive (indicating matrix elements). To avoid capillary pressure scaling while maintaining permeability scaling in a particular element (see Section A.2.4), the desired PMX is multiplied by 10^{-30} . Then the code uses internally the correct PMX value for flow computation, while bypassing permeability scaling.

A.5. DATA BLOCK TRACR

This is a new data block required by EOS9NT V2.0. It provides all the necessary information on the tracers and their treatment. It includes the following cards:

A.5.1. Card TRACR.1

The following information is provided in TRACR. 1:

NTRACR, MXTRDT, NOITTR, FLOWFI, LPLACE,
LPTYPE, NITR, CRLAPL, NOPRNT

according to the format

FORMAT (3 (I5) , 4X, A6 , I1 , A4 , I2 , 3X, E10 . 4 , I2)

These parameters are defined as follows:

- | | |
|--------|--|
| NTRACR | The number of tracers. If ITRACR \neq 0 in PARAM. 1 and ITRACR \neq NTRACR, then a warning message will be printed and the simulation will be aborted. |
| MXTRDT | The maximum allowable number of time steps in the solute transport simulation. It refers to the highest number from among all the tracers. If MXTRDT is left blank, it is reset to 99999. If MXTRDT \neq 0 but MXTRDT < MCYC, then MXTRDT is reset to MXTRDT = MXTRDT+MCYC . |
| NOITTR | The maximum allowable number of Newtonian iterations for the solution of the transport equation (applies for conventional time stepping only). If NOITTR is left blank, it is reset to 5. |
| FLOWFI | The status of the flow field. If FLOWFI='steady', then the flow equation is solved only once to obtain the required velocities and mass fluxes across the element connections. Only the solute equations are then solved. If FLOWFI \neq 'steady', FLOWFI is reset internally to 'transi', and both the flow and transport equations are solved. |
| LPLACE | If LPLACE=1, then, after the flow field becomes time-invariant, the transport equations are solved using a Laplace transform formulation. For LPLACE \neq 1, conventional timestepping is employed in the solution of the |

tracer equations.

LPTYPE The algorithm for the numerical inversion of the Laplace space solutions. There are two option:
LPTYPE = 'stfs' : The Stehfest algorithm is used
LPTYPE = 'hoog' : The Hoog algorithm is used
If LPTYPE≠'stfs', LPTYPE≠'hoog' and LPLACE= 1, a warning is printed and the simulation is aborted

NITR The number of summation terms in the algorithms for the numerical inversion of the Laplace space solutions.

For LPTYPE='stfs', NITR is an even integer, and $10 \leq NITR \leq 18$. If $NITR < 10$ or $NITR > 18$, or is left blank, it is reset internally to the default value of 18. If an odd number between 10 and 18 is entered, NITR is reset internally to the next larger integer value.

For LPTYPE='hoog', NITR is an integer, and $5 \leq NITR \leq 10$. If $NITR < 5$, $NITR > 10$, or is left blank, it is reset internally to the default value of 6.

CRLAPL The convergence criterion for the conjugate gradient solution in the Laplace space. Because a very accurate solution must be obtained in the Laplace space to ensure accurate solutions in time, the convergence criterion must be much tighter than for the flow equation. If $CRLAPL > 10^{-9}$, $CRLAPL < 10^{-14}$, or is left blank, it is reset internally to the default value of 10^{-10} .

NOPRNT If $NOPRNT \neq 0$, only the mass and volume balances of phases and tracers are printed. Otherwise, the distributions in the domain are also printed (default $NOPRNT = 0$). This is a useful feature for breakthrough studies in very large grids.

If $NTRACR=0$, no additional cards are read in the TRACR data block, and the simulation is conducted without considering any tracers, i.e., only the flow equation is solved. Note that, if $NTRACR=0$, a TRACR data block is not necessary.

A.5.2. Card TRACR.2

The following variables are read in TRACR. 2:

IFFACT, ISFACT, IDFACT, ICOVRD, ITOVRD, ICOURAN, HLFACR, BoundB, QConcB

according to the format

FORMAT (5 (I1, 1X), 2 (E10.4)), A2, 1X, A1

These parameters are defined as follows:

IFFACT Indicator for flow velocity averaging (default IFFACT=0). It is not applicable

when the Laplace transform formulation is invoked.

IFFACT=0: The flow velocity is interpolated at the midpoint of the transport $\Delta t_{t,i}$.

IFFACT=1: The flow velocity is interpolated at the end of the transport $\Delta t_{t,i}$.

IFFACT=2: The flow velocity is interpolated at the midpoint of the flow Δt_f .

IFFACT=3: The flow velocity is interpolated at the end of the flow Δt_f .

ISFACT Indicator for water saturation averaging (default ISFACT=0). It is not applicable when the Laplace transform formulation is invoked.

ISFACT=0: The water saturation is interpolated at the midpoint of the transport $\Delta t_{t,i}$.

ISFACT=1: The water saturation is interpolated at the end of the transport $\Delta t_{t,i}$.

ISFACT=2: The water saturation is interpolated at the midpoint of the flow Δt_f .

ISFACT=3: The water saturation is interpolated at the end of the flow Δt_f .

IDFACT Indicator for radioactive decay averaging (default IDFACT=0). It is not applicable when the Laplace transform formulation is invoked.

IDFACT=0: The decay is applied to the tracer concentration at the end of the transport $\Delta t_{t,i}$ (default).

IDFACT=1: The decay is applied to the tracer concentration at the midpoint of the transport $\Delta t_{t,i}$.

ICOVRD Indicator for overriding the default Courant number (the default value of ICOVRD=0). It is not applicable when the Laplace transform formulation is invoked.

ICOVRD \neq 9: The Courant number is reset to the default (=1) if it exceeds 1.

ICOVRD=9: The Courant number is not reset to the default (=1) if it exceeds 1, but the value in COURAN is used.

ITOVRD Indicator for overriding the default half-life fraction for $\Delta t_{t,i}$ limitation (default ITOVRD =0). It is not applicable when the Laplace transform formulation is invoked.

ITOVRD \neq 9: The half-life fraction is reset to the default (=0.1) if it exceeds 0.1.

ITOVRD=9: The half-life fraction is reset to the default (=0.1) if it exceeds 0.1, but the value in HLFAC is used.

COURAN The maximum allowable Courant number (default COURAN = 1.0). It is not applicable when the Laplace transform formulation is invoked. If COURAN \leq 0 or

COURAN > 1, COURAN is reset to COURAN = 1.0. If COURAN > 1 and ICOVRD = 9, COURAN is not reset but remains as specified.

HLFRAC The maximum allowable fraction of the tracer half-life (if radioactive) for limiting $\Delta t_{i,i}$ (default HLFAC = 0.1). It is not applicable when the Laplace transform formulation is invoked. If HLFAC ≤ 0 or HLFAC > 0.1, HLFAC is reset to HLFAC = 0.1. If HLFAC > 0.1 and ITOVRD=9, HLFAC is not reset but remains as specified.

BoundB A 2-character variable that describes the decay behavior of the tracer concentration at the domain boundaries. It is not needed when studying stable isotopes. BoundB can have one of three values. When BoundB = 'CT' (default) the concentration at all the boundaries remains constant over time, i.e., new, 'freshly-made' radionuclide continuously enters the domain from the boundaries; thus, a radionuclide that has migrated deep into the formation has experienced far more pronounced decay than radionuclides that only recently entered the system. If left blank, BoundB is internally reset to the default value of 'CT'.

When BoundB = 'DT', the concentration at all the various boundaries is temporally variable as the species undergoes radioactive decay. Thus, the radionuclide residing at the boundaries is treated as having been produced all at the same time. When BoundB = 'VT', the temporal behavior of concentration is not uniform, and element-specific information on the temporal behavior of concentration must be provided in the data block INCON or INDOM. In this case, some boundary gridblocks can have constant release of 'fresh' radionuclide, while others release radionuclides at time-variable (decaying) concentrations.

Note that the variability discussed in conjunction with BoundB is related strictly to radioactive decay, and not to possible temporal fluctuations of release rate. EOS9NT V2.0 then calculates internally the time-variable concentrations at the boundaries for all members of any radioactive chain.

QConcB A single-character variable that describes the decay behavior of the radionuclides at the various sources (injection points) only (not needed when studying stable isotopes). QConcB is entirely analogous to BoundB, and can have one of three values. When QConcB = 'C' (default), the concentration at all the injection points constant over time, i.e., new, 'freshly-made' radionuclide is continuously injected.

When QConcB = 'D', the concentration at all the various sources declines with time as the species undergoes radioactive decay. When BoundB = 'VT', the temporal behavior of concentration is not uniform, and element-specific information on the temporal behavior of concentration in each injection point must be provided in the data block GENER.

A.5.3. Cards TRACR.3.1, TRACR.3.1.1, TRACR.3.2, and TRACR.3.3

These are read according to the following format:

```
do n=1,NTRACR
  read TRACR.3.1
  if TRTYPE='SI', then:
    if TRTYPE='TC' or 'PC', read TRACR.3.1.1
  do i=1,NMROCK (on Card TRACR.3.1 - defined below)
    read TRACR.3.2
    read TRACR.3.3
    read TRACR.3.4
    if TRTYPE='SC', read TRACR.3.5
  end do
end if
end do
```

The parameters on card TRACR.3.1 are:

TRACER, TRTYPE, PCTYPE, NMROCK, IDROCK, NDAUTR, NADDID,
IDPARE, IDSEQ, MATCOL, DD00, HAFLIF, WTMOL, X Ref

and the corresponding format is

```
FORMAT(A5,A2,A1,6(i3),4x,4(e10.4))
```

A.5.3.1. The parameters in Card TRACR.3.1.

These are defined as follows:

- TRACER The tracer name.
- TRTYPE The type of tracer. For pseudocolloids, TRTYPE='PC'; for true colloids, TRTYPE='TC'; for solutes not involved in sorption onto colloids, TRTYPE='SO' (default); for solutes sorbed irreversibly onto colloids, TRTYPE='SI'; and for solutes involved that sorb reversibly onto colloids, TRTYPE='SC'.
- PCTYPE PCTYPE = 'P': Designates a decaying radioactive precursor. This designation is reserved for the initial precursor modeled for a given decay chain.
- PCTYPE = 'D': Designates a radioactive decay product
- PCTYPE = 'S': Pertains to colloids only, and designates colloid-assisted transport
- PCTYPE = 'N': Non-radioactive substance, or no colloid assisted transport
- NMROCK The number of domains for which sorption coefficients are provided.
- IDROCK If NMROCK is less than the total number of domains in the data block ROCKS, then the properties of the remaining domains will be set equal to those of the domain with the IDROCK sequence number (i.e., the order in which the rock type

is read in the data block ROCKS). If IDROCK \leq 0 or IDROCK > number of rock domains, the domains about which no sorption data are provided are assumed to be non-sorbing.

NDAUTR	Number of decay products. It is necessary if PCTYPE='P'.
NADDID	This is needed only in colloid-assisted radionuclide transport (i.e., when TRTYPE='SC' or 'SI'), and is tracer number of the colloid involved in such transport (and onto which the solutes sorb).
IDPARE	Precursor identifier, indicating the tracer number of the parent of a radioactive or reactive chain. It is necessary if PCTYPE='D'.
IDSEQ	The decay sequence number of the decay product in the radioactive decay chain. It is necessary if PCTYPE='D'.
DD00	The tracer molecular diffusion coefficient (m ² /s). In colloids, this value is replaced by an internally computed estimate of the colloid diffusion coefficient based on the colloid diameter and the water temperature. See Equation (3-25)
HAFLIF	The tracer half life (s). If the field is left blank, HAFLIF is reset internally to the default (= 10 ⁵⁰ s). If HAFLIF<0 and PCTYPE='P' or PCTYPE='D', ABS (HAFLIF) is the reaction constant.
WTMOL	The molecular weight of the tracer. It is necessary if the daughter of the tracer is tracked.
X_Ref	A reference mass fraction. The highest possible concentration in the domain can be used as X_Ref. It is introduced to improve the accuracy of computations by reducing roundoff error effects when the initial mass fraction levels are very small. Setting X_Ref = 1.0 has no effect on the computations, but X_Ref = 0.0 will cause an error message to be printed and the simulation to stop. X_Ref is very important in the case of colloid-assisted transport with solutes irreversibly sorbed onto colloids (TRTYPE = 'SI'). In this case, X_Ref is the initial radionuclide mass ratio in the colloid, computed as the mass of the radionuclide to the mass of the radionuclide-free pseudocolloid. Then X_Ref is the only source of information on the radionuclide concentration in the colloids, and overrides any other information in the data blocks PARAM, INCON or INDOM. Note that a solution of EOS9NT V2.0 is only possible if BoundB = 'DT' and QConcB = 'D', in which case the same decay effect affects uniformly the radionuclides on all colloids. If TRTYPE = 'SI', card TRACR.3.1 is the last input card needed for that tracer.

A.5.3.2. The parameters in Card TRACR.3.1.1.

For colloid filtration (TRTYPE='TC' or 'PC'), the card TRACR.3.1 is followed by card TRACR.3.1.1, which includes the parameters

COLDIA (n) , RHOCOL (n) , I VarFv (n)

These are read according to the format

FORMAT (2 (e10.4) , i2)

and are defined as follows:

COLDIA (n)	The diameter d_c (in m) of colloid n. If COLDIA<0 and the colloid n is a true colloid (TRTYPE = 'TC') and radioactive, EOS9NT V2.0 will perform the transport simulations by using a time-variable d_c that decreases with decay. The decreasing d_c affects the colloid diffusion coefficient D_0 and the colloid accessibility factor f_c .
RHOCOL (n)	The density ρ_c (in kg/m ³) of colloid n.
I_VarFv (n)	A flag describing the treatment of the colloid velocity adjustment factor f with a decreasing colloid diameter d_c due to radioactive decay. For I_VarFv<0, f is continuously adjusted internally.

A.5.3.3. The parameters in Card TRACR.3.2.

A total of NMROCK cards TRACR.3.2 are read. The parameters on the cards are:

NNROCK, NSORTP (NNROCK, n, 1) , NSORTP (NNROCK, n, 2) ,
NSORTP (NNROCK, n, 2) , NOSAME (NNROCK)
(SKD (NNROCK, n, j) , j=1, . . . , 6) , DDSS (NNROCK, n)

and the corresponding format is

FORMAT (I3 , 1X, I1 , I1 , 1X, I3 , 7 (e10.4))

where n is the tracer number for which sorption and filtration parameters are read. These parameters are defined as follows:

NNROCK	The sequence number of the rock domain, of which the sorption properties will be read immediately after.
NSORTP (NNROCK, n, 1):	A flag indicating the type of sorption of tracer n on the rock/soil i. = 1: Linear equilibrium sorption (physical) = 2: Langmuir equilibrium sorption (physical) = 3: Freundlich equilibrium sorption (physical) = 4: Linear kinetic sorption (physical) = 5: Langmuir kinetic sorption (physical) = 6: Freundlich kinetic sorption (physical) = 7: Linear kinetic chemical sorption = 8: Colloid equilibrium filtration

= 9: Colloid kinetic filtration and declogging

NSORTP (NNROCK, n, 2): A flag indicating the presence of combined sorption of solute n on the rock/soil NNROCK. NSORTP (NNROCK, 2) = 0 indicates no combined sorption or filtration. Otherwise, it denotes the second type (secondary) of the combined sorption or filtration.

= 1: Linear equilibrium sorption (physical)

= 2: Langmuir equilibrium sorption (physical)

= 3: Freundlich equilibrium sorption (physical)

= 4: Linear kinetic sorption (physical)

= 5: Langmuir kinetic sorption (physical)

= 6: Freundlich kinetic sorption (physical)

= 7: Linear kinetic chemical sorption

= 8: Colloid equilibrium filtration

= 9: Colloid kinetic filtration and declogging

NOSAME (NNROCK) The number of additional rock/soil domains that have the same properties with domain NNROCK. If NOSAME (NNROCK) $\neq 0$, then the domain numbers of NOSAME (NNROCK) additional rocks/soils will be read in card(s) TRACR. 3.3 immediately after the card TRACR. 3.2.

DDSS The tracer surface diffusion coefficient (m^2/s). DDSS is reset internally to DDSS=0 when the tracer is a colloid (PCTYPE='PC' or 'TC').

Defining $N_1 = NSORTP ((NNROCK, n, 1))$,

SKD (NNROCK, n, 1) For $N_1 = 1$ or 4 K_d (in m^3/kg): distribution coefficient of the linear equilibrium sorption of tracer n onto domain number NNROCK.

For $N_1 = 2$ or 5 K_1 (in m^3/kg): coefficient of the Langmuir equilibrium sorption of tracer n onto domain number NNROCK.

For $N_1 = 3$ or 6 K_F (in m^b/kg^{3b}): coefficient of the Freundlich equilibrium sorption of tracer n onto domain number NNROCK.

For $N_1 = 7$ k_c^+ (in $1/s$): the forward kinetic coefficient of the chemical sorption of solute n onto domain number NNROCK.

	For $N_1 = 8$	K_σ (in m^3/kg): distribution coefficient of the linear equilibrium deposition of colloid n onto domain number NNROCK
	For $N_1 = 9$	κ^+ (in $\text{m}^3/\text{kg}/\text{s}$): kinetic clogging coefficient of filtration (attachment) of colloidal tracer n to domain number NNROCK – see equation (13). This value is used only when the corresponding flag KCOMOD \leq 3.
SKD (NNROCK, n , 2)	For $N_1 = 1, 8$	Set to zero internally (not used).
	For $N_1 = 4$	δ_p (dimensionless): a parameter determining if the primary kinetic sorption is irreversible.
	For $N_1 = 2$ or 5	K_2 (in m^3/kg): coefficient of the Langmuir equilibrium sorption of tracer n onto domain number NNROCK.
	For $N_1 = 3$ or 6	b (dimensionless): exponent of the Freundlich equilibrium sorption of tracer n onto domain number NNROCK
	For $N_1 = 7$	k_c^- (in 1/s): the backward kinetic coefficient of the chemical sorption of solute n onto domain number NNROCK.
	For $N_1 = 9$	For KCOMOD(...,1) = 1 (Section I.5.3.4). If SKD(...,2)<0, the kinetic declogging coefficient is computed internally as $\kappa^- = \delta_p \kappa^+ R_\kappa$, where $R_\kappa = \kappa^- / \kappa^+$. If SKD(...,2)>0, then $\kappa^- = \delta_p \kappa$, where κ is provided by SKD(...,3).
	For $N_1 = 9$	For KCOMOD=2, SKD(...,2) is the kinetic declogging coefficient κ^- (in 1/s).
	For $N_1 = 9$	For KCOMOD= 3, 4, 5, 6. If SKD(...,2)<0, it is the constant ratio

$R\hat{\epsilon}$, and $\kappa^- = \kappa^+ R_{\kappa}$. If $SKD(\dots,2) > 0$,
 $SKD(\dots,2) = \kappa^-$ (in 1/s).

SKD (NNROCK, n, 3)	For $N_1 = 1,2,3,7,8$	Set to zero internally (not used).
	For $N_1 = 4$	k_{ℓ} (in 1/s): the kinetic constant of the linear kinetic sorption of tracer n onto domain NNROCK
	For $N_1 = 5$	k_L (in 1/s): kinetic constant of the Langmuir kinetic sorption of tracer n onto domain NNROCK.
	For $N_1 = 6$	k_F (in 1/s): kinetic constant of the Freundlich kinetic sorption of tracer n onto domain number NNROCK.
	For $N_1 = 9$	$k = \kappa^-$ (in 1/s): kinetic declogging coefficient of filtration of colloidal tracer n through domain number NNROCK – used only when $KCOMOD(\dots,1) = 1$.

The parameters SKD (NNROCK, n, 4), SKD (NNROCK, n, 5) and SKD (NNROCK, n, 6) describe the same parameters as SKD (NNROCK, n, 1), SKD (NNROCK, n, 2) and SKD (NNROCK, n, 3), respectively, and pertain to $N_2 = NSORTP ((NNROCK, n, 2))$, i.e., to the secondary sorption or infiltration.

A.5.3.4. The parameters in Card TRACR.3.3 for colloid transport.

For colloid transport (TRTYPE= 'TC' or 'PC'), the card TRACR. 3 . 2 is followed by card TRACR . 3 . 2 . 1, which includes the parameters

ALPHAL (NNROCK, n) , ALPHAT (NNROCK, n) , TRANCO (NNROCK, n) ,
 COVLFA (NNROCK, n) , COLEFF (NNROCK, n) , ENTRFR (NNROCK, n) ,
 KCOMOD (NNROCK, n, 1) , KCOMOD (NNROCK, n, 2)

These are read according to the format

FORMAT (6 (E10.4) , 1x, i1, 1x, i1)

and are defined as follows:

ALPHAL (NNROCK, n) The longitudinal dispersivity α_L (in m) of colloid n in rock NNROCK.

ALPHAT (NNROCK, n) The transverse dispersivity α_T (in m) of colloid n in rock

NNROCK. ALPHAL and ALPHAT may depend on the colloidal particle size.

- TRANCO (NNROCK, n) The transfer coefficient K_i (see Equation 3-16 and 3-17).
- COVLFA (NNROCK, n) The velocity adjustment factor f of colloid n in rock NNROCK. If COVLFA >1.5 or COVLFA <1 , it is reset internally to 1 (default). When the colloid is a radioactive true colloid (TRTYPE='TC') and $I_VarFv < 0$, COVLFA is computed internally and is continuously adjusted to reflect the effects of the decreasing colloid diameter.
- COLEFF (NNROCK, n) The single collector efficiency α_c of colloid n in rock NNROCK.
- ENTRFR (NNROCK, n) The accessibility factor f_c of colloid n in rock NNROCK. When the colloid is radioactive true colloid (TRTYPE = 'TC') and COLDIA <0 (see Section I.5.3.2), ENTRFR is computed internally and is continuously adjusted to reflect the effects of the decreasing colloid diameter.
- KCOMOD (NNROCK, n, 1) A flag describing the model to be used to compute the primary filtration coefficients when the filtration of colloid n is described by a kinetic model, i.e., when NSORTP(NNROCK,n,1)=9. The following options are possible:
- KCOMOD (NNROCK, n, 1)=1: The κ^+ parameter— see Equation (3-17) — is obtained from the corresponding SKD(NNROCK,n,1); the κ^- parameter is obtained as a function of κ^+ and of the corresponding SKD(NNROCK,n,2).
- KCOMOD (NNROCK, n, 1)=2: The κ^+ parameter is obtained from SKD(NNROCK,n,1); the κ^- parameter is fixed and is given by SKD(NNROCK,n,2).
- KCOMOD (NNROCK, n, 1)=3: The κ^+ parameter is obtained according to the *Dieulin* [1982] model from the corresponding SKD(NNROCK,n,3); the $\hat{\epsilon}$ - parameter is obtained as a function of κ^+ and of the corresponding SKD(NNROCK,n,2).
- KCOMOD (NNROCK, n, 1)=4: This option pertains to colloid filtration in fractures only. In this case, the κ^+ parameter is obtained according to the *Abdel-Salam and Chysikopoulos* [1994] model from the corresponding SKD(NNROCK,n,3); the κ^- parameter is obtained as a function of κ^+ and of the corresponding SKD(NNROCK,n,2).

KCOMOD(NNROCK, n, 1)=5: The κ^+ parameter is obtained according to the Yao *et al.* [1971] model from various input parameters; the κ^- parameter is obtained as a function of κ^+ and of the corresponding SKD(NNROCK, n, 2).

KCOMOD(NNROCK, n, 1)=6: The κ^+ parameter is obtained according to the Tien *et al.* [1979] model from various input parameters; the κ^- parameter is obtained as a function of κ^+ and of the corresponding SKD(NNROCK, n, 2).

KCOMOD(NNROCK, n, 2) A flag describing the model to be used to compute the secondary filtration coefficients when the filtration of colloid is described by a kinetic model, i.e., when NSORTP(NNROCK, n, 2)=9. It is entirely analogous to KCOMOD(NNROCK, n, 1).

A.5.3.5. The parameters in Card TRACR.3.3 for solute transport.

For solute transport (TRTYPE='SO' or 'SC'), the card TRACR.3.2.1, includes the parameters

ALPHAL(NNROCK, n), ALPHAT(NNROCK, n), TRANCO(NNROCK, n)

These are read according to the format

FORMAT(6(E10.4), 1x, i1, 1x, i1)

and are as defined in Section I.5.3.4.

A.5.3.6. Options for describing filtration in EOS9NT V2.0.

Equilibrium filtration in EOS9NT V2.0 is handled by setting N_1 (and N_2 , if secondary filtration is considered) to 8.

A.5.3.7. The parameters in Card TRACR.3.4.

The parameters on card TRACR.3.3 are:

(NOROCK(NNROCK, j), j=1, ..., NOSAME(NNROCK))

and the corresponding format is

FORMAT(16(I5))

NOROCK is the domain number of rocks/domains that have the same properties with domain NNROCK.

A.5.3.8. The parameters in Card TRACR.3.5.

This card is only needed when the tracer is a solute involved in colloid-assisted transport through reversible sorption onto colloids (TRTYPE='SC'. Then card TRACR.3.5 includes the following parameters:

NSORTP (nnrkmx, n, 1) , SKD (nnrkmx, n, 1) , SKD (nnrkmx, n, 2) ,
SKD (nnrkmx, n, 3) , TRANCO (nnrkmx, n)

and the corresponding format is

FORMAT (I1, 4x, 7 (E10.4))

These parameters have been previously defined (see Section A.5.3.3). In this case, they describe the sorption of the solute tracer *n* onto the colloid defined by the NADDID(*n*) parameter (see Section A.5.3.1). Only primary sorption onto the colloid is allowed. Note that these properties are assigned to a fictitious 'rock' that corresponds to the maximum rock number. This indicates that, under these conditions, nnrkmx must be larger than the number of actual rocks present in the system (see Section A.1).

A.5.3.9. Important issues.

The Laplace transform formulation can only be applied when sorption is described by a linear equilibrium or kinetic process. Therefore, if the input data define non-linear conditions while a Laplace formulation is invoked (LPLACE=1), EOS9NT V2.0 resets LPLACE to zero, a warning message is printed, and conventional time stepping is employed. In preparing the data set TRACR, the user must keep in mind that the order of listing of the tracers is important because it defines the computation order of the solutions for each of the tracers. The data cards of the members of a radioactive decay or reaction chain must be listed consecutively. This is because EOS9NT stores the solutions of the parents for the computation of the solutions of the daughters. Because of the sequential nature of the tracer solutions in EOS9NT, the stored solution from the previous species will not correspond to the correct daughter if parents and daughters are not in order.

If the study includes solutes and colloid-assisted transport on more than one type of pseudocolloid, it is important to first list the cards with the parameters of all the colloids, and follow them with the cards with the solute properties.

A.6. DATA BLOCK INCON

A.6.1. Card INCON.1

The computational parameters read in INCON.1 are:

EL, NE, NSEQ, NADD, PORX, KTRACR, B_time

and the format is

FORMAT(A3,I2,2I5,E15.8,I2,1x,a1)

All the parameters in INCON.1 are as defined in [Pruess, 1987; 1991]. The new parameter KTRACR= *n*, i.e., the number of tracers under consideration. If KTRACR (≠0) differs from NTRACR in the data block TRACR in Section A.4, a warning of the discrepancy is printed and the simulation is aborted.

The other new parameter `B_time` is a single-character variable that describes the decay behavior in the element. It is used only when (a) the element in question is a boundary element (i.e., one whose properties and conditions do not change over time), (b) the species is radioactive, and (c) `BoundB = 'VT'` in the block `PARAM` (denoting spatial variability in the decay behavior of the boundary elements).

`B_time` can have two values. When `B_time = 'C'` (default) the concentration at all the boundaries remains constant over time, i.e., new, 'freshly-made' radionuclide is continuously available at the element. If left blank, `B_time` is internally reset to the default value of 'C'. When `B_time = 'D'`, the concentration at the boundary element is temporally variable as the species undergoes radioactive decay.

A.6.2. Cards `INCON.2`

This card is the same as in `EOS9` (Pruess et al. 1999), and lists the primary variable describing the hydraulic state of the system, i.e., either the water saturation (under two-phase conditions), or the pressure (under single-phase conditions).

A.6.3. Cards `INCON.3`, `INCON.4` and `INCON.5`

These new cards (or sets of cards, if the number of tracers ≥ 4) `INCON.3` and `INCON.4` read the (a) initial mass fractions of the tracers, (b) the initial primary sorbed or filtered (for colloids) concentrations (in kg/m^3), and (c) the initial secondary sorbed or filtered (for colloids) concentrations (in kg/m^3), respectively, i.e.,

```

TMASSF ( I ) , I=1 , . . . , max { NTRACR , ITRACR }
XSOFIL ( I ) , I=1 , . . . , max { NTRACR , ITRACR }
XSOFI2 ( I ) , I=1 , . . . , max { NTRACR , ITRACR }

```

according to the format

```

FORMAT ( 4E20.13 )

```

If colloid-assisted solute transport involving reversible sorption onto colloids is studied (`TRTYPE='SC'`), then only primary sorption of the solute onto the porous medium can be considered. In this case, `XSOFI2` represents the solute sorbed onto the sum of mobile and immobile (filtered) colloids, expressed as kg of solute per unit bulk volume). The use of `max { NTRACR , ITRACR }` is necessitated by the ability of `TOUGH2` to read the input data blocks in an arbitrary order. Thus, there is no guarantee that the number of tracers will have been read in `PARAM` (`ITRACR`) or `TRACR` (`NTRACR`) when the `INCON` data are read. Although this approach provides an extra level of redundancy, there is still a possibility of a problem if `INCON` is read before the `PARAM` and `TRACR` data blocks. Thus, it is important to ensure that these data blocks are read before `INCON`. Note that in `EOS9NT V2.0` all the equations are linear with respect to concentration for `LE` or `LKP` sorption/filtration. Thus, under these conditions, any value can be used as the initial `TMASSF`, to be changed later by multiplying by an appropriate factor. It is convenient to use `TMASSF=1`.

A.7. DATA BLOCK INDOM

A.7.1. Card INDOM.1

The computational parameters read in INDOM.1 are:

NAM, KTRACR

and the format is

FORMAT (A5, I2)

The parameter NAM in INDOM.1 is as defined in [Pruess, 1987; 1991]. The parameter KTRACR= n , i.e., the number of tracers under consideration. If KTRACR($\neq 0$) differs from NTRACR in the data block TRACR in Section A.4, a warning of the discrepancy is printed and the simulation is aborted.

A.7.2. Cards INDOM.3, INDOM.4 and INDOM.5

These new cards (or sets of cards, if the number of tracers ≥ 4) INDOM.3 read (a) initial mass fractions of the tracers, (b) the initial primary sorbed or filtered (for colloids) concentrations, and (c) the initial secondary sorbed or filtered (for colloids) concentrations (for combined sorption), respectively, i.e.,

TMASIN(I), I=1, ..., max{NTRACR, ITRACR}
XSOFIN(I), I=1, ..., max{NTRACR, ITRACR}
XSOF2N(I), I=1, ..., max{NTRACR, ITRACR}

according to the format

FORMAT (4E20.13)

If colloid-assisted solute transport involving reversible sorption onto colloids is studied (TRTYPE='SC'), then XSOF2N represents the solute sorbed onto the sum of mobile and immobile (filtered) colloids, expressed as kg of solute per unit bulk volume). Because of the reasons discussed in the previous section (4.5), it is important to ensure that the PARAM and TRACR data blocks are read before INDOM.

A.8. DATA BLOCK GENER

A.8.1. Card GENER.1

This card is modified to read the following parameters:

EL, NE, SL, NS, NSEQ, NADD, NADS, LTAB, TYPE, ITAB
GX, EX, HX, NTRQ, Q_time

according to the format

FORMAT (A3, I2, A3, I2, 4I5, 5X, A4, A1, 3E10.4, I2, 1x, a1)

NTRQ and Q_time are the only additions, with all other parameters remaining as defined in

Pruess [1987]. NTRQ is the number of tracers, and is only important if GX \geq 0.0, i.e., only for injection. NTRQ is internally checked against NTRACR and ITRACR, and the simulation is aborted (after printing a warning message) if a discrepancy is detected. The other new parameter Q_time is a single-character variable that describes the decay behavior. It is used only when (a) a source is involved (i.e., injection is occurring), (b) the species is radioactive, and (c) QConcB = 'V' in the block PARAM (denoting spatial variability in the decay behavior of the various sources). Q_time can have two values. When Q_time = 'C' (default) the concentration at all the sources remains constant over time, i.e., new, 'freshly-made' radionuclide is continuously available at the injection stream. If left blank, Q_time is internally reset to the default value of 'C'. When Q_time = 'D', the concentration in the injection stream is temporally variable as the species undergoes radioactive decay.

A.8.2. Card GENER.1.0.1

This new card (or cards, if NTRQ \geq 4) is (are) read immediately after GENER.1 only when GX \geq 0.0, and includes the parameters.

$$\text{TMFQ}(I), \quad I=1, \dots, \text{NTRQ}$$

These are read according to

$$\text{FORMAT}(4\text{E}20.13)$$

The parameter TMFQ(I) is the mass fraction of tracer I in the injection stream when TMFQ(I) > 0. When it has a negative value, ABS(TM FQ(I)) represents the actual mass injection rate of tracer I in kg/s.

A.8.3. Card GENER.1.3

The heat equation is not solved in EOS9NT V2.0. The GENER.1.3 card (or cards) is (are) thus used to read the mass fractions of the tracers in the injection streams in a tabular form, i.e.,

$$\text{F3}(L), \quad L=1, \dots, \text{NTRACR} * \text{LTAB}$$

according to

$$\text{FORMAT}(4\text{E}14.7)$$

If the declared size of F3 is insufficient, then a warning message is printed and the simulation is aborted. An important point is that to implement the Laplace transform formulation, the injection mass rate GX must be constant over time. If GX is time-variant, the Laplace transform formulation can still be employed if its time dependence can be described by a time function with a known Laplace transform. In this case, however, the user will have to modify subroutine LQTRCR (for the Stehfest algorithm) and/or HQTRCR (for the De Hoog algorithm) by adding the code for the Laplace transform of the injection rate.

A.9. OPTIONS FOR VERY LARGE GRIDS

When the grid exceeds 100,000 elements, problems arise if the conventional TOUGH2 options [Pruess, 1991] are employed. These problems surface when TOUGH2 creates the external MESH and GENER files for subsequent transport simulations involving the same domain and source/sink set.

A.9.1. Problems in the MESH File

After reading the element and connection data, TOUGH2 creates the MESH file, at the end of which it attaches the indices of the elements in all the grid connections. These indices allow computational economy in subsequent runs because TOUGH2 does not spend the time needed for their determination (a considerable task in large grids). The conventional TOUGH2 writes these indices according to a standard `FORMAT(16(I5))` format. For grids $\geq 100,000$ elements, this format is inadequate because larger fields are required. Thus, the created MESH file is erroneous and cannot be further used.

A.9.2. Problems in the GENER File

A similar problem arises in the creation of GENER. After reading the element names at which sinks and sources are located, conventional TOUGH2 determines the corresponding element numbers and attaches them at the end of the GENER file using the same standard `FORMAT(16(I5))`. In large grids involving a large number of sources, the associated computational effort is significant. The corresponding time savings by reading (rather than determining) the source/sink element numbers from the GENER file cannot be realized when the grid $\geq 100,000$ elements because their numbers are incorrectly stored.

A.9.3. Addressing the Problems When `No_CEN=5`

When `No_CEN=5` (i.e., when 5-character element names are used), the problem is eliminated by attaching the `ext1` keyword at the end of the `ELEME` and `GENER` keywords. Thus, the new keywords at the top of the `ELEME` and `GENER` data blocks become `ELEMEext1` and `GENERext1`, respectively. When EOS9NT V2.0 reads the `ext1` keyword, the element indices at the end of the MESH and GENER files are stored according to `FORMAT(10(I8))` instead of the standard `FORMAT(16(I5))`.

These keywords cause the parameters

```
ELEM, MA1, MA2, VOLX, AHTX, ZREF, X, Y, Z
```

in the Card `ELEME.1` of the `ELEME` data block (see Section A.4.1) to be read and written according to

```
FORMAT(A5, 10X, A3, A2, 3E10.4, 2F10.3, F10.4)
```

A.9.4. Addressing the Problems When `No_CEN=8`

When `No_CEN=8` (i.e., when 8-character element names are used), very large problems become tractable. By using this approach, the problem is eliminated by attaching the `ext2` keyword at

the end of the ELEM, CONNE and GENER keywords. Note that if there is a conflict between No_CEN=5 and ext2, a warning message is printed and the simulation is aborted. Thus, the new keywords at the top of the ELEM, CONNE and GENER data blocks become ELEMext2, CONNEext2 and GENERext2, respectively. When No_CEN=8 and EOS9NT V2.0 reads the ext2 keyword, these keywords cause the following:

(a) In Card ELEM.1 of the ELEM data block (see Section A.4.1), the following parameters

```
EL6_0, NE, MA1, MA2, VOLX, AHTX, zref, X, Y, Z
```

are read and written according to

```
FORMAT(A6, I2, 7X, A3, A2, 3E10.4, 3F10.3)
```

The parameter EL6_0 is the 6-character component of the element name, analogous to the EL parameter in 5-character names (see Section A.9.3).

(b) In Card CONNE.1 of the CONNE data block [Pruess, 1987;1991], the following parameters

```
EL6_1, NE1, EL6_2, NE2, ISOT, D1, D2, AREAX, BETAX
```

are read and written according to

```
FORMAT(A6, I2, A6, I2, 9X, I5, 4E10.4)
```

The parameters EL6_1 and EL6_2 are the 6-character components of the names of the connection, analogous to the EL1, EL2 parameters in 5-character names.

(c) The element indices at the end of the MESH and GENER files are stored according to

```
FORMAT(10(I8)).
```

(d) In Card GENER.1 of the GENER data block, the following parameters

```
EL6_0, NE, SL, NS, LTAB, TYPE, ITAB, GX, EX, HX, ntrqqq, Q time
```

are read and written according to

```
FORMAT(A6, I2, A3, I2, 12X, I5, 5X, A4, A1, 3E10.4, I2, 1X, A1)
```

The parameter EL6_0 is the 6-character component of the element name, analogous to the EL parameter in 5-character names (see Section A.8.1).

(e) In Card INCON.1 of the INCON data block, the following parameters

```
EL6_0, NE, PORX, ktracr, B_time
```

are read and written according to

```
FORMAT(A6, I2, 7X, E15.8, I2, 1X, A1)
```

The parameter EL6_0 is the 6-character component of the element name, analogous to the

EL parameter in 5-character names (see Section A.6.1).

ATTACHMENT B. OUTPUT DATA

EOS9NT V2.0 will provide the following output:

- 1) The standard general information outputs of the TOUGH2 family of codes (Pruess, 1991) includes parameter setting in the main program, an documentations on permeability modification, on the setting of the MOP-parameters for choosing program options, and on the time-stepping information.
- 2) The options and general tracer transport information data blocks ROCKS, PARAM, and TRACR of Attachment A.
- 3) The pressure (in Pa), saturation, capillary pressure (in Pa), the relative permeability and diffusivity(m^2/s) of the liquid phase in the gridblocks of the domain.
- 4) The flux (in kg/s)and velocity (in m/s) of the liquid phase across the grid block interfaces (connections) of the domain.
- 5) The primary variable (pressure or saturation) and its changes in the gridblocks of the domain.
- 6) The mass fractions of the n tracers in the water phase (in kg/kg), and the corresponding physically and chemically sorbed (for solutes) or filtered (for colloids) concentrations (in kg/m^3 of medium), as well as (c) the reacted mass fractions in the water phase (in kg/kg) in the gridblocks of the domain.
- 7) The diffusive, advective and total fluxes of the n tracers (in kg/s) across the gridblock interfaces of the domain.
- 8) Volume and mass balances of the liquid and gas phases in the domain (in m^3 and kg, respectively), and mass balances of the n tracers (in kg).
- 9) The standard output files printed by TOUGH2 V1.11. The output includes flow output (OUT in flow chart: Attachment C) and transport outputs which can be TOUT (traditional time stepping), HTOUT (Laplace Transform and De Hoog method), and LTOUT (Laplace Transform and Stehfest Method)
- 10) The output file VELOC which includes velocity data.
- 11) The output file UNVEC which includes the unit vector data.
- 12) The output file INDEX which includes the indices of neighboring domain cells.

Of those possible outputs, (1), (2), (8) and (9) are to be always to be printed. In keeping with the TOUGH2 convention, if the KDATA values are increased by 10, printouts shall occur after each iteration (not just after convergence).

Note that when the flow field is or becomes time-invariant, (3), (4) and (5) shall be printed only once. After this point, only the transport equations shall be solved, and thus only the transport outputs (6), (7) and (8) are to be printed.

ATTACHMENT C. FLOW CHART

