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EOS7R: Radionuclide Transport for TOUGH2

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Abstract

EOS7R provides radionuclide transport capability for TOUGH2. EOS7R extends the EOS7 module (water, brine, and optional air) to model water, brine, parent component, daughter component, and optional air and heat. The radionuclide components follow a first-order decay law, and may adsorb onto the solid grains. Volatilization of the decaying components is modeled by Henry's Law. The decaying components are normally referred to as radionuclides, but they may in fact be any trace components that decay, adsorb, and volatilize. The decay process need not be radioactive decay, but could be any process that follows a first-order decay law, such as biodegradation. EOS7R includes molecular diffusion for all components in gaseous and aqueous phases using a simplified binary diffusion model. When EOS7R is used with standard TOUGH2, transport occurs by advection and molecular diffusion in all phases. When EOS7R is coupled with the dispersion module T2DM, one obtains T2DMR, the radionuclide transport version of T2DM. T2DMR models advection, diffusion, and hydrodynamic dispersion in rectangular two-dimensional regions. Modeling of radionuclide transport requires input parameters specifying the half-life for first-order decay, distribution coefficients for each rock type for adsorption, and inverse Henry's constants for volatilization. Options can be specified in the input file to model decay in "inactive" grid blocks and to read from standard EOS7 INCON files. We present a number of example problems to demonstrate application and accuracy of TOUGH2/EOS7R. One-dimensional simulation results agree well with analytical solutions. For a two-dimensional salt-dome flow problem, the final distribution of daughter radionuclide component is complicated by the presence of weak recirculation caused by density effects due to salinity.

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1. Introduction

EOS7R extends the equation of state module EOS7 (for water, brine, and optional air and heat) to include parent and daughter radionuclide components. Additional subroutine modifications extend the standard TOUGH2 process description to include first-order decay, equilibrium sorption, molecular diffusion in aqueous and gas phases, and volatilization of the radionuclide components. Transport of the five components (water, brine, parent radionuclide, daughter radionuclide, and air) is by advection and molecular diffusion. When EOS7R is coupled with the dispersion module T2DM, the process description is further extended to include Fickian hydrodynamic dispersion. However, whereas TOUGH2/EOS7R can model advection and diffusion in arbitrary irregular 1-, 2-, and 3-dimensional grids, modeling of hydrodynamic dispersion with T2DMR is restricted to two-dimensional rectangular cartesian domains. We refer to the combination of T2DM and EOS7R as T2DMR. This report describes EOS7R, the model for radionuclide transport, and its optional coupling with T2DM. The sample problems and input format descriptions in the present report provide sufficient information to use EOS7R, the new TOUGH2 module for radionuclide transport. For details of the brine process description, users are referred to the EOS7 report (Pruess, 1991b). The foundations and instructions for use of the dispersion module (T2DM) are described in Oldenburg and Pruess (1993).

2. Mathematical Formulation

2.1. *General*

The general conservation equations solved by the integral finite difference method (IFDM) in TOUGH2 consist of balances between mass accumulation and flux and source terms over all grid blocks V_n into which the flow domain V has been partitioned:

$$\frac{\mathrm{d}}{\mathrm{dt}}\int_{V_n} M^{(\kappa)}\,\mathrm{d}V = \int_{\Gamma_n} \mathbf{F}^{(\kappa)}\cdot\mathbf{n}\quad \mathrm{d}\Gamma + \int_{V_n} q^{(\kappa)}\,\mathrm{d}V \qquad (1)$$

(see Nomenclature for definition of symbols). In Eq. 1, the index n = 1, ..., N corresponds to the grid blocks with volume V_n and surface area Γ_n . The index κ = 1, ..., NK+1 corresponds to the NK fluid components and heat. The mass accumulation term (M) in Eq. 1 is given by

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

The flux term has contributions from both the phase flux and from diffusion and dispersion and can be written

$$\mathbf{F}^{(\kappa)} = \sum_{\beta=1}^{NPH} \left(X_\beta^{(\kappa)} \mathbf{F}_\beta - \rho_\beta \overline{\mathbf{D}}_\beta^{(\kappa)} \nabla X_\beta^{(\kappa)} \right) \qquad (3).$$

The first term on the right-hand side of Eq. 3 is the phase flux term which accounts for the flux of component κ arising from Darcy flux of the phases containing κ. The second term on the right-hand side of Eq. 3 is the dispersion term with the dispersion tensor indicated by the overbar. When EOS7R is coupled with T2DM, hydrodynamic dispersion is modeled with a Fickian formulation that includes transversal and longitudinal dispersion for all components (see Oldenburg and Pruess (1993) for details). Without the T2DM subroutines, EOS7R models molecular diffusion only.

EOS7R can handle 2 phases and 5 components plus heat. The symbols and index numbers for these phases and components in EOS7R are shown in Table 1. Air and heat are optional components, the consideration of which is specified in the MULTI block of the input file (see section 4.3)

Table 1. Phases and components in EOS7R.

Phases (β)	Components (κ)				
1 – gas (g)	1 – water	2 – brine	3 – parent	4 – daughter	5 – air
2 – aqueous (w)	1 – water	2 – brine	3 – parent	4 – daughter	5 – air

2.2 *Molecular Diffusion*

We use a simplified model for binary diffusion of the chemical components dissolved in aqueous and gas phases. The bold $\overline{\mathbf{D}}$ in Eq. 3 is the dispersion tensor, a second order, symmetric tensor with one principal direction in the average (Darcy) flow direction, and the other normal to it. The dispersion tensor of Eq. 3 can be written as

$$\overline{\mathbf{D}}_{\beta}^{\kappa} = D_{T,\beta}^{\kappa}\ \overline{\mathbf{I}} + \frac{\left(D_{L,\beta}^{\kappa} - D_{T,\beta}^{\kappa}\right)}{u_{\beta}^{2}}\mathbf{u}_{\beta}\,\mathbf{u}_{\beta} \qquad (4).$$

The strength of dispersion is specified by dispersion coefficients in the longitudinal (D_L) and transverse (D_T) directions relative to the flow direction where

$$D_{L,\beta}^{\kappa} = \phi\ S_{\beta}\ \tau\ \ d_{\beta}^{\kappa} + \alpha_L\, u_{\beta} \qquad (5)$$

$$D_{T,\beta}^{\kappa} = \phi\ S_{\beta}\ \tau\ \ d_{\beta}^{\kappa} + \alpha_T\, u_{\beta} \qquad (6).$$

Here ϕ is the porosity, S_{β} is the saturation of phase β, τ is the tortuosity of the medium, d_{β}^{κ} is the molecular diffusivity for component κ in phase β, α_L is the longitudinal dispersivity, or longitudinal dispersion length, α_T is the transverse dispersivity, and u_{β} is the magnitude of the Darcy velocity of phase β. In the modified subroutines provided with EOS7R, we neglect hydrodynamic dispersion, assuming effectively that α_L and α_T are zero. (If hydrodynamic dispersion is to be modeled, users must link subroutines in T2DM with EOS7R and provide additional input parameters, details of which are presented in Sections 4.1 and 4.2). With the assumption that $\alpha_L = \alpha_T = 0$, the dispersion tensor contains only isotropic molecular diffusion, specifically,

$$\overline{\mathbf{D}}_\beta^\kappa = \phi \, S_\beta \, \tau \;\; d_\beta^\kappa \; \overline{\mathbf{I}} \tag{7}$$

where $\overline{\mathbf{I}}$ is the identity matrix. Substituting Eq. 7 into Eq. 3 gives the mass flux of component κ due to molecular diffusion in phase β:

$$\mathbf{F}_{\beta,d}{}^{(\kappa)} = -\rho_\beta \, \overline{\mathbf{D}}_\beta^{(\kappa)} \nabla X_\beta^{(\kappa)} = -\rho_\beta \, \phi \, S_\beta \, \tau \;\; d_\beta^\kappa \, \nabla X_\beta^{(\kappa)} \tag{8}$$

This term is added to the phase flux (first term in Eq. 3) to form the total flux for component κ. In addition to modification by $S \tau$, gas-phase diffusivities are affected by temperature and pressure as in TOUGH and TOUGH2 (Pruess, 1987, 1991a), except that temperature dependence is neglected by default, and non-zero TEXP must be input to turn on temperature dependence. The diffusion model as given in Eqs. 7 and 8 approximates multicomponent diffusion as composed of binary pairs. Such an approximation is applicable if one component is dominant (e.g., water) while the others are dilute. We caution the user that the full details of multicomponent diffusion (e.g., Cussler, 1984, Chap. 8) are not captured by the present simplified effective binary diffusion model.

2.3 *Adsorption*

In EOS7R, the radionuclide components ($\kappa = 3,4$) in the aqueous phase may be adsorbed onto the immobile solid grains of the matrix. Our development follows that of deMarsily (1986, p. 256) and assumes that the amount of a species that is adsorbed is proportional to its concentration in the aqueous phase. If the adsorbing component κ is sufficiently dilute, then its adsorption does not affect adsorption of any of the other components present. With this assumption, the adsorption of component κ can be described by the distribution coefficient, Kd, where

$$Kd_w^{(\kappa)} = \frac{f^{(\kappa)}}{c_w^{(\kappa)}} \tag{9}$$

and where

$$f^{(\kappa)} = \frac{mass\ of\ component\ \kappa\ adsorbed}{mass\ of\ solid} \tag{10}$$

$$c_w^{(\kappa)} = \frac{mass\ of\ component\ \kappa}{volume\ of\ aqueous\ phase\ (w)} \tag{11}.$$

With the assumption of local equilibrium, $f^{(\kappa)}$ may also be expressed in terms of the gas-phase concentration of component κ,

$$f^{(\kappa)} = Kd_w^{(\kappa)}\, c_w^{(\kappa)} = Kd_g^{(\kappa)}\, c_g^{(\kappa)} \tag{12}.$$

Thus there is an effective Kd for the gas phase related to Kd_w by Henry's constant (see section 2.5). The mass accumulation term of Eq. 2 including the effect of adsorption then becomes

$$M^{(\kappa)} = \phi \sum_{\beta=1}^{NPH} S_\beta \rho_\beta X_\beta^{(\kappa)} + (1 - \phi)\rho_R f^{(\kappa)} \tag{13}.$$

Selecting the aqueous liquid phase (w) as a reference phase, the mass accumulation term can be written relative to the reference phase (w):

$$M^{(\kappa)} = \phi \sum_{\beta=1}^{NPH} S_\beta \rho_\beta X_\beta^{(\kappa)} + (1 - \phi)\rho_R c_w^{(\kappa)} Kd_w^{(\kappa)} \tag{14}.$$

In Eq. 14, the contribution to the mass accumulation term due to adsorbed component κ is expressed relative to the reference phase (w), with solute concentration given by

$$c_w^{(\kappa)} = \rho_w X_w{}^{(\kappa)} \tag{15}$$

and distribution coefficient $Kd_w^{(\kappa)}$.

To relate the above multiphase formulation to the customary retardation factor formulation for single-phase systems, we consider a system in which component κ partitions only between the aqueous phase and the solid grains (i.e., component κ is non-volatile, or gas phase is absent). Isolating the terms for the reference phase (w), Eq. 14 can be written

$$M^{(\kappa)} = \phi S_w \rho_w X_w{}^{(\kappa)} \left(1 + \frac{(1 - \phi)}{\phi S_w} \rho_R K d_w^{(\kappa)} \right) \tag{16}$$

where the terms in parentheses comprise the retardation factor (R). Rather than using the retardation factor as an input parameter, we implement adsorption in EOS7R by specifying distribution coefficients for the reference phase (w) for each rock type. Nevertheless, for comparison with analytical solutions of fully saturated flow problems which often use R as a parameter, we will present some later results in terms of the retardation factor, R. The effective aqueous phase retardation factor for full multiphase partitioning is given by

$$R_w^{(\kappa)} = 1 + \frac{(1\text{-}\phi)}{\phi\, S_w} \rho_R K d_w{}^{(\kappa)} + \sum_{\beta \neq w} \frac{S_\beta\, \rho_\beta\, X_\beta{}^{(\kappa)}}{S_w\, \rho_w\, X_w{}^{(\kappa)}} \qquad (17).$$

2.4. *First-Order Decay*

The radionuclide components ($\kappa = 3$ or 4, the parent and daughter components, respectively) may undergo radioactive decay by a first-order decay law

$$\frac{d}{dt} M_l^{(\kappa)} = -\lambda_\kappa M_l^{(\kappa)} \qquad (18)$$

where $M_l^{(\kappa)}$ is the mass of species κ per unit volume in subdomain l, and λ_κ is the radioactive decay constant of component κ, related to the half-life by

$$T_{1/2} = \frac{ln\ 2}{\lambda_\kappa} \qquad (19).$$

The implementation of first-order decay into the IFDM in TOUGH2 can be explained as follows. First, we rewrite Eq. 1 in space-discretized form as an ordinary differential equation (ODE) in time for grid block l,

$$\frac{d}{dt} V_l M_l^{(\kappa)} = \sum_m A_{lm} F_{lm}^{(\kappa)} + q_l^{(\kappa)} V_l \qquad (20),$$

where m labels the grid blocks connected to l and where the source term accounts for radioactive decay. Substituting Eq. 18 for the sink term in Eq. 20, we obtain

$$\frac{d}{dt} V_l M_l^{(\kappa)} = \sum_m A_{lm} F_{lm}^{(\kappa)} - \lambda_\kappa M_l^{(\kappa)} V_l \qquad (21).$$

Introducing time-step index k and iteration index p, we can now write the time-discretized equation for the decaying parent component ($\kappa = 3$) as

$$M_l^{(3)\,k+1,\ p} - M_l^{(3)\,k} = \frac{\Delta t}{V_l} \sum_m A_{lm} F_{lm}^{(3)\,k+1,\ p} - \lambda_3\ \Delta t\ M_l^{(3)\,k+\Phi,\,p} \qquad (22)$$

where we use a variable time-weighting parameter (Φ) for the decay term. The source-sink term (last term on the right-hand side of Eq. 22) that accounts for radioactive decay depends on the mass at the ($k + \Phi$) time level. We introduce a simple interpolation scheme to approximate the mass accumulation term at the $k + \Phi$ level as follows:

$$M_l^{(\kappa)\, k+\Phi,\ p} = M_l^{(\kappa)\, k} + \Phi\left(M_l^{(\kappa)\, k+1,\ p} - M_l^{(\kappa)\, k}\right) \qquad (23).$$

Fully implicit differencing for the decay term corresponds to $\Phi = 1$, and Crank-Nicholson (mid-point) weighting corresponds to $\Phi = 0.5$. Upon substitution of Eq. 23 into 22 and rearranging, we obtain

$$M_l^{(3)\, k+1,\ p}\left(1 + \Phi\,\lambda_3\,\Delta t\right) - M_l^{(3)\, k}\left(1 - \left(1 - \Phi\right)\lambda_3\,\Delta t\right) = \frac{\Delta t}{V_l}\sum_m A_{lm} F_{lm}^{(3)\, k+1,\ p} \qquad (24).$$

The default for the decay term in TOUGH2/EOS7R is the fully implicit scheme ($\Phi = 1.$). If the half-life is input as a negative number, Φ is assumed to equal 0.5 (Crank-Nicholson) which makes the source term that accounts for radioactive decay be the average of the radionuclide mass at the old (k) and current ($k + 1$) time steps. When concentration changes occur primarily due to flow and transport, $\Phi = 1$ is recommended (fully implicit). When decay is the dominant mechanism for concentration change, $\Phi = 0.5$ will give more accurate results.

The mass accumulation term for radionuclide component 4 (the daughter) includes production by decay of component 3 (the parent) and destruction by its own decay:

$$\frac{d}{dt} M_l^{(4)} = -\lambda_4 M_l^{(4)} + \lambda_3 M_l^{(3)} \frac{MW^{(4)}}{MW^{(3)}} \qquad (25).$$

The ratio of molecular weights enters Eq. 25 because the decay reactions occur on a per-mole basis while we write the conservation equations on the basis of mass balance. We will show later that in many applications this distinction is unimportant (see sample problems). Substituting Eq. 25 into the ODE for the conservation of daughter component, we obtain

$$\frac{d}{dt} V_l M_l^{(4)} - V_l M_l^{(3)} \frac{MW^{(4)}}{MW^{(3)}} \lambda_3 = \sum_m A_{lm} F_{lm}^{(4)} - \lambda_4 M_l^{(4)} V_l \qquad (26)$$

which is analogous to Eq. 21 for the parent. We can rearrange Eq. 26 to obtain

$$\frac{d}{dt} V_l M_l^{(4)} + \lambda_4 V_l M_l^{(4)} - \lambda_3 V_l M_l^{(3)} \frac{MW^{(4)}}{MW^{(3)}} = \sum_m A_{lm} F_{lm}^{(4)} \qquad (27).$$

Introducing time step index k, time-weighting parameter Φ, and iteration index p, we now write the time-discretized equation for the daughter component:

$$\begin{gathered} M_l^{(4)\,k+1,\,p} \left(1 + \Phi \lambda_4 \Delta t\right) - M_l^{(4)\,k} \left(1 - \left(1 - \Phi\right) \lambda_4 \Delta t\right) - \\ \lambda_3 \Delta t \left[M_l^{(3)\,k+1,\,p} \Phi - M_l^{(3)\,k} \left(1 - \Phi\right)\right] \frac{MW^{(4)}}{MW^{(3)}} = \frac{\Delta t}{V_l} \sum_m A_{lm} F_{lm}^{(4)\,k+1,\,p} \end{gathered} \qquad (28).$$

As for the parent, the daughter half-life may be input as a positive number (for $\Phi = 1$, fully implicit), or as a negative number (for $\Phi = 0.5$, mid-point weighting). Note that input of either parent or daughter half-lives as negative numbers will impose $\Phi = 0.5$ for both parent and daughter.

The above models for molecular diffusion, adsorption, and radioactive decay have been coded in a revised subroutine MULTI distributed with EOS7R. With the addition of these new processes, new input parameters are required, specifications for which are discussed in section 4.3. Because radionuclide concentrations are expected to be very low, thermal effects of radioactive decay have been neglected. The formulation developed here is sufficiently general that first-order decay processes other than radioactive decay can also be modeled with EOS7R (e.g., see sample problem 2).

2.5 *Volatilizaton*

In addition to adsorbing onto solid matrix grains, the radionuclide components may volatilize into the gas phase, if present. This volatilization is represented under conditions of local thermodynamic equilibrium by Henry's Law:

$$P_g^{(\kappa)} = H_{gw}^{(\kappa)} \chi_w^{(\kappa)} \qquad (\kappa = 3,4) \tag{29}$$

where $P_g^{(\kappa)}$ is the partial pressure in the gas phase of component κ, $H_{gw}^{(\kappa)}$ is Henry's constant, and $\chi_w^{(\kappa)}$ is the mole fraction of component κ in the aqueous phase. Consistent with existing TOUGH2 formulations for water and air, we specify volatilization with inverse Henry's constants ($1/H_{gw}^{(\kappa)}$), which are actually solubilities (units of Pa^{-1}). Although adsorption is specified by a distribution coefficient for the aqueous phase only, there is an effective distribution coefficient for the gas phase that arises from the partitioning between the aqueous and gaseous phases. Assuming that the gas phase consists primarily of air, the effective gas-phase distribution coefficient can be written in the following approximate form:

$$Kd_g^{(\kappa)} = \frac{f^{(\kappa)}}{\rho_g \dfrac{H_{gw}^{(\kappa)} \chi_w^{(\kappa)}}{P_g} \dfrac{MW^{(\kappa)}}{MW^{(a)}}} \tag{30}$$

This effective $Kd_g^{(\kappa)}$ is never explicitly calculated or used in EOS7R. We mention it only to make the point that retardation occurs for volatile species in the gas phase just as it does in the aqueous phase, even if there is no explicit distribution coefficient for the gas phase.

In EOS7R as in EOS7, no solubility constraints are enforced for the brine (Pruess, 1991b). Users are cautioned that unphysical results may be obtained in thermal problems with strong vaporization effects.

3. Implementing Radionuclide Transport

The implementation of the above processes involved extending the EOS7 thermophysical properties module (Pruess, 1991b) to include two radionuclide components that partition into the gas phase, as well as adding molecular diffusion, adsorption, and first-order decay to subroutine MULTI. EOS7R refers to both the new equation of state module and the associated revised subroutines (e.g., MULTI). The number of components is specified in the MULTI block of the input file. The order of the components in EOS7R is water, brine, radionuclide 1 (parent), radionuclide 2 (daughter), air (if present), and heat (if present) (Table 1). A summary of EOS7R specifications is printed upon execution and is reproduced here in Fig. 1.

Because EOS7R adds two new components to EOS7, two additional equations must be solved. Linear equation solution can become quite slow for large problems with up to 6 equations per grid block (5 mass components and heat). For faster linear equation solution, EOS7R uses T2CG1, which provides the choice of 3 conjugate gradient solvers specified through the MOP(21) option (Moridis and Pruess, 1995). The radionuclide components are often at very low concentration and can be treated as tracer components. As such, they do not affect the flow field. There may be times when users will want to compute, for example, a steady-state flow field with strong brine density effects without the added computational overhead of the radionuclide transport. Once a steady-state flow field is obtained, the user may want to study the transport of the radionuclides within the steady flow field. We have allowed for this type of execution through appropriate specification of the MOP(19) option. If MOP(19) is set equal to 1, EOS7R will expect to read a standard EOS7 INCON format (up to 4 primary variables, i.e. no radionuclides). For MOP(19) equal to 0 (the default), the INCON block is assumed to be in EOS7R format (up to 6 primary variables). These options also apply to the primary variables specified in PARAM.4.

```
*****************************************************************************************************************************
*     EOS7R:  EQUATION OF STATE FOR MIXTURES OF WATER/BRINE/RADIONUCLIDE(1)/RADIONUCLIDE(2)/AIR                             *
*****************************************************************************************************************************

   OPTIONS SELECTED ARE: (NK,NEQ,NPH,NB) = (4,4,2,10)

                         NK  =  4   - NUMBER OF COMPONENTS
                         NEQ =  4   - NUMBER OF EQUATIONS PER GRID BLOCK
                         NPH =  2   - NUMBER OF PHASES THAT CAN BE PRESENT
                         NB  = 10   - NUMBER OF SECONDARY PARAMETERS (OTHER THAN COMPONENT MASS FRACTIONS)

   AVAILABLE OPTIONS: (5,5,2,11) - WATER, BRINE, RN1, RN2, AIR; ISOTHERMAL (DEFAULT); VARIABLES (P, XB, XRN1, XRN2, X OR S+10, T)
                      (5,6,2,11) - WATER, BRINE, RN1, RN2, AIR; NON-ISOTHERMAL;       VARIABLES (P, XB, XRN1, XRN2, X OR S+10, T)
                      (4,4,2,10) - WATER, BRINE, RN1, RN2, NO AIR; ISOTHERMAL;        VARIABLES (P, XB, XRN1, XRN2, T)
                      (4,5,2,10) - WATER, BRINE, RN1, RN2, NO AIR; NON-ISOTHERMAL;    VARIABLES (P, XB, XRN1, XRN2, T)

   THE NK = 4 ("NO AIR") OPTIONS MAY ONLY BE USED FOR PROBLEMS WITH SINGLE-PHASE LIQUID CONDITIONS THROUGHOUT.

   THE NORMAL NUMBER OF SECONDARY PARAMETERS OTHER THAN MASS FRACTIONS IS 6 PER PHASE.  IN EOS7R, WE ADD TO THIS ONE MOLECULAR
   DIFFUSIVITY FOR EACH POTENTIAL COMPONENT IN EACH PHASE MAKING NB = 10 OR 11.
*****************************************************************************************************************************

THE PRIMARY VARIABLES ARE
 P - PRESSURE    T - TEMPERATURE     XB - BRINE MASS FRACTION IN LIQUID (FOR SINGLE-PHASE GAS, XB IS BRINE MASS FRACTION IN GAS)
 XRN1 - MASS FRACTION IN THE LIQUID OF RADIONUCLIDE(1) (PARENT)   XRN2 - MASS FRACTION IN THE LIQUID OF RADIONUCLIDE(2) (DAUGHTER)
 S+10. - (GAS PHASE SATURATION + 10.)    X - AIR MASS FRACTION     T - TEMPERATURE

******************************                               ****************************************************************
*        COMPONENTS          *                               *   FLUID PHASE CONDITION           PRIMARY VARIABLES          *
******************************                               ****************************************************************
*                            *                               *                                                              *
*       # 1  -  WATER        *                               *   SINGLE-PHASE GAS (#)            P, XB, XRN1, XRN2,     X, T *
*                            *                               *                                                              *
*       # 2  -  BRINE        *                               *   SINGLE-PHASE LIQUID (*)         P, XB, XRN1, XRN2,     X, T *
*                            *                               *                                                              *
*       # 3  -  RN1          *                               *   TWO-PHASE (*)                   P, XB, XRN1, XRN2, S+10., T *
*                            *                               *                                                              *
*       # 4  -  RN2          *                               ****************************************************************
*                            *                                (#) SINGLE-PHASE GAS NOT FULLY IMPLEMENTED.
*       # 5  -  AIR          *                                (*) XRN1 AND XRN2 ARE ALWAYS MASS FRACTIONS IN THE AQUEOUS PHASE.
*                            *
*       # 6  -  HEAT         *
*                            *
*****************************************************************************************************************************

NEGATIVE REFERENCE PRESSURE OF  -.100000E+06 PA WAS SPECIFIED, THUS BRINE PROPERTIES ARE IDENTICAL TO WATER FOR ALL SALINITIES.

PROPERTIES OF THE RADIONUCLIDES:   DOMAIN     RADIONUCLIDE(1)           RADIONUCLIDE(2)
          HALF-LIFE (SECONDS):      -ALL-       .1728E+07                 .1000E+41
   MOLECULAR WEIGHT (GM/MOLE):      -ALL-       .2340E+03                 .2300E+03
INVERSE HENRY CONST.(MOLE/PA):      -ALL-       .1000E+31                 .1000E+31
GAS PHASE DIFFUSIVITY (M**2/S):     -ALL-       .0000E+00                 .0000E+00
AQ. PHASE DIFFUSIVITY (M**2/S):     -ALL-       .1157E-06                 .0000E+00
DISTRIBUTION COEFF. (M**3/KG):      FINE        .1620E-03                 .0000E+00

MOLECULAR DIFFUSIVITY OF WATER, BRINE, XRN1, XRN2, AND AIR THROUGH THE GASEOUS AND AQUEOUS PHASES, (FDDIAG(PHASE,COMP)) [M**2/S]:
PHASE 1 = GAS;  PHASE 2 = AQUEOUS
  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP
   -1-  -1-    -1-  -2-    -1-  -3-    -1-  -4-    -1-  -5-    -2-  -1-    -2-  -2-    -2-  -3-    -2-  -4-    -2-  -5-
  .00000E+00  .00000E+00  .00000E+00  .00000E+00  .00000E+00  .11570E-06  .00000E+00  .11570E-06  .00000E+00  .00000E+00

  MOP(19) = 0 *** ALLOWS INITIALIZATION WITH DIFFERENT SETS OF PRIMARY VARIABLES. ***
               *** THIS IS USEFUL FOR STARTING EOS7R SIMULATIONS FROM EOS7 INITIAL CONDITIONS. ***
          = 0: (P,XB,XRN1,XRN2,XAIR,T) FOR SINGLE PHASE, (P,XB,XRN1,XRN2,S+10,T) FOR TWO-PHASE.  (EOS7R FORMAT).
          = 1: (P,XB,XAIR,T) FOR SINGLE PHASE, (P,XB,S+10,T) FOR TWO-PHASE.  (EOS7 FORMAT).  WILL INITIALIZE XRN1 = XRN2 = 0.

*****************************************************************************************************************************
```

Fig. 1. Example of self-documenting printout for EOS7R.

Special consideration must be given to decay and production of radionuclides in grid blocks which are given very large volume so that their thermodynamic conditions remain approximately constant. Users can choose to allow for the radionuclide to decay within very large grid blocks, or the user can choose to have a constant mass of radionuclide within such blocks. The two options are selected on the basis of the volume of the grid block. If the volume of the grid block is larger than or equal to 1.E50 m^3, then the mass fractions of the radionuclides will be unchanged from their initial values. If the volume of a grid block is less than 1.E50 m^3, the mass fractions will change by radioactive decay and production as they would in any other grid block.

4. Using EOS7R

4.1. *Compilation of EOS7R*

As an extension of TOUGH2, EOS7R consists of all of the TOUGH2 subroutines, some with modifications, and the new equation of state module EOS7R itself. The program units and their changes for radionuclide transport are presented in Appendix 1. A typical compilation instruction on an IBM RS/6000, for example, would be as follows:

xlf -O -qautodbl=dblpad *eos7r.f* t2cg1.f t2f.f meshm.f ma28.f

The italics indicate the new program units for radionuclide transport. Note that duplicate subroutine name warnings may arise from some compilers. Depending on the compiler, it is possible that duplicate main programs and subroutines may have to be eliminated from the source code. Alternatively, one can change the names of later occurrences of the same subroutine (e.g., an unwanted version of CYCIT could be renamed CYCITx).

4.2. *Compilation of T2DMR*

To model hydrodynamic dispersion, it is necessary to link subroutines from the dispersion module, T2DM. The additional program units needed are described in Appendix 2.

The compilation instruction on an IBM RS/6000 would be:

xlf -O -qautodbl=dblpad *t2dmr.f* *eos7r.f* t2cg1.f t2f.f meshm.f ma28.f

Again, italics indicate new program units, and duplicate subroutines may have to be eliminated for some compilers.

4.3 *Input Formats*

Below we describe the input formats for adsorption and radioactive decay. All other TOUGH2 input parameter formats are given in Pruess (1987) and Pruess (1991a). The input parameters for diffusion, adsorption, radioactive decay, and volatilization in EOS7R are provided through the SELEC block and two new parameters in the ROCKS block. Some input is needed only by T2DMR and is labeled accordingly in the descriptions below. Note that records containing only dispersion input (e.g., SELEC.4) must still be present, although the actual input variable fields can be left blank.

MULTI format(4I5)

NK, NEQ, NPH, NB

NK	Number of components. Set NK = 4 for water, brine, parent, and daughter. Set NK = 5 for water, brine, parent, daughter, and air.
NEQ	Number of equations per grid block. Set NEQ = NK for isothermal problems. Set NEQ = NK + 1 for nonisothermal problems.
NPH	Number of phases. Set NPH = 2.
NB	Number of secondary parametes. Set NB = NK + 6 for six secondary parameters plus one molecular diffusivity for each component.

PARAM.1 format(2I2, 3I4, 24I1, 2E10.4)

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

See TOUGH report (Pruess, 1987), TOUGH2 informative printout, and the T2DM report (Oldenburg and Pruess, 1993) for description of all of the above parameters except the following:

MOP(19) Selects type of INCON format;

0: INCON file or INCON block is in EOS7R format.

1: INCON file or INCON block is in standard EOS7 format. All radionuclide components are initialized with $X^{(\kappa)} = 0$.

MOP(21) Selects type of linear equation solver;

0: defaults to DSLUCS (Bi-conjugate gradient (Lanczos type) with incomplete LU factorization).

1: Direct solver MA28.

2: DSLUBC (Bi-conjugate gradient with incomplete LU factorization).

3: DSLUCS (Bi-conjugate gradient (Lanczos type) with incomplete LU factorization).

4: DSLUGM (Generalized minimum residual conjugate gradients with incomplete LU factorization).

DIFF0 Not used in EOS7R.

TEXP Exponent for temperature dependence in gas-phase diffusivity equation as described in TOUGH manual. Must be non-zero to activate temperature-dependent gas-phase diffusivity.

ROCKS keyword to introduce material parameters.

ROCKS.1.1 format(8E10.4)

COM, EXPAN, CDRY, TORTX, GK, XKD3, XKD4

TORTX Tortuosity factor. If input as zero or blank, molecular diffusive fluxes are not calculated for that material.

XKD3 Distribution coefficient for parent radionuclide, component 3, in the aqueous phase, $m^3\ kg^{-1}$.

XKD4 Distribution coefficient for daughter radionuclide, component 4, in the aqueous phase, $m^3\ kg^{-1}$.

(See Pruess (1987, 1991a) for description of other ROCKS input parameters)

SELEC keyword to introduce a data block with reference brine, geometry, dispersion, and radioactive decay data.

SELEC.1 format(8I5)

IE(1), NGBINP(1), NGBINP(2), NGBINP(3), NFBL, NFBR, NFBT, NFBB

IE(1) set equal to 6 to read six additional data records of brine, geometry, dispersion and decay data.

The 7 input variables following IE(1) are for T2DMR only and can be left blank if T2DMR is not used.

NGBINP(1) number of grid blocks in X (must always be equal to 1).

NGBINP(2) number of grid blocks in Y.

NGBINP(3) number of grid blocks in Z.

NFBL number of the first ("left") column of grid blocks within the flow domain (defaults to 1 if zero or blank).

NFBR	number of the last ("right") column of grid blocks within the flow domain (defaults to NGBINP(2) if zero or blank).
NFBT	number of the first ("top") row of grid blocks within the flow domain (defaults to 1 if zero or blank).
NFBB	number of the last ("bottom") row of grid blocks within the flow domain (defaults to NGBINP(3) if zero or blank).

SELEC.2 format(3E10.4)

P_0, T_0, ρ_b

P_0	reference pressure, Pa.
T_0	reference temperature, °C.
ρ_b	brine density at (P_0,T_0), kg m^{-3}.

For P_0, T_0, and ρ_b equal to zero or blank, default values of $P_0 = 1 \times 10^5$ Pa, $T_0 = 25$ °C, $\rho_b = 1185.1$ kg m^{-3} will be used. If $P_0 < 0$, brine will have the same thermophysical properties as pure water (see EOS7 User's Guide; Pruess, 1991b)

SELEC.3 format(3E10.4)

v(i), i=1,3

v(i)	coefficients for salinity correction in aqueous phase viscosity (see EOS7 User's Guide; Pruess, 1991b). For v(i) = 0, default values will be used. Specification of pure water in record SELEC.2 will override viscosity specifications.

SELEC.4 format(2E10.4)

ALPHAT, ALPHAL

The following 2 input variables are for T2DMR only.

ALPHAT	transverse dispersivity, m.
ALPHAL	longitudinal dispersivity, m.

SELEC.5 format(6E10.4)

FDDIAG(NP,NK), NK=1,2,5; NP=1,2

FDDIAG(NP,NK)	Molecular diffusivities: first diffusivity for water, brine, and air in phase 1 (gas), then diffusivity for water, brine, and air in phase 2 (aqueous) (see Table 2). Note that the tortuosity of each material in the ROCK block of the input file must be set to some non-zero value to model molecular diffusion effects. If FDDIAG(NP,NK) is input as a negative number, the absolute value is used for the phase molecular diffusivity (d_β^κ) of Eqs. 5 and 6 without modification by S and τ (saturation and tortuosity) and without pressure or temperature effects in the case of gas diffusivity.

SELEC.6 format(7E10.4)

XHALF(3), XMW(3), (FDDIAG(NP,NK), NK=3; NP=1,2), blank, blank, HCRN1

XHALF(3)	half-life of parent radionuclide, component 3, in seconds.
XMW(3)	molecular weight of component 3, in g/mole.
FDDIAG(NP,3)	Molecular diffusivity of component 3 in phase 1 (gas), followed by molecular diffusivity of component 3 in phase 2 (aqueous). If FDDIAG(NP,3) is input as a negative number, the absolute value is used for the phase molecular diffusivity (d_β^κ) of Eqs. 5 and 6 without modification by S and τ (saturation and tortuosity) and

without pressure or temperature effects in the case of gas diffusivity.

HCRN1 — inverse Henry's constant for parent radionuclide, Pa^{-1}.

SELEC.7 format(7E10.4)

XHALF(4), XMW(4), (FDDIAG(NP,NK), NK=4; NP=1,2), blank, blank, HCRN2

XHALF(4) — half-life of daughter radionuclide, component 4, in seconds.

XMW(4) — molecular weight of component 4, in g/mole.

FDDIAG(NP,4) — Molecular diffusivity of component 4 in phase 1 (gas), followed by molecular diffusivity of component 4 in phase 2 (aqueous). If FDDIAG(NP,4) is input as a negative number, the absolute value is used for the phase molecular diffusivity (d_β^κ) of Eqs. 5 and 6 without modification by S and τ (saturation and tortuosity) and without pressure or temperature effects in the case of gas diffusivity.

HCRN2 — inverse Henry's constant for daughter radionuclide, Pa^{-1}.

Table 2. Molecular diffusivities for two phases and five components.

phase	component	(NP,NK)	input	units
gaseous	water	(1,1)	FDDIAG(1,1)	$m^2\ s^{-1}$
	brine	(1,2)	FDDIAG(1,2)	$m^2\ s^{-1}$
	air	(1,5)*	FDDIAG(1,5)*	$m^2\ s^{-1}$
	rn1	(1,3)	FDDIAG(1,3)	$m^2\ s^{-1}$
	rn2	(1,4)	FDDIAG(1,4)	$m^2\ s^{-1}$
aqueous	water	(2,1)	FDDIAG(2,1)	$m^2\ s^{-1}$
	brine	(2,2)	FDDIAG(2,2)	$m^2\ s^{-1}$
	air	(2,5)*	FDDIAG(2,5)*	$m^2\ s^{-1}$
	rn1	(2,3)	FDDIAG(2,3)	$m^2\ s^{-1}$
	rn2	(2,4)	FDDIAG(2,4)	$m^2\ s^{-1}$

* the order of listing diffusivities reflects the order in input file. See SELEC.5, 6, and 7.

5. Example Problems

5.1. *One-Dimensional Radionuclide Transport with Adsorption and Decay*

In this section, we present two variations of an example problem of one-dimensional radionuclide transport with adsorption and radioactive decay. The first variation considers the one-dimensional transport of radionuclides in a homogeneous saturated porous medium of porosity 30% with a steady flow field of 0.1 m/day pore velocity. The results are compared to analytical solutions for verification. The second variation considers the same problem with two-phase conditions. The problem domain is shown in Fig. 2.

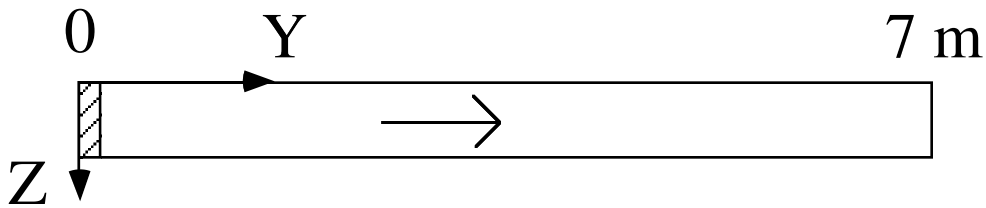

Fig. 2. Domain for one-dimensional transport problem.

In the first variation, transport is by advection and hydrodynamic dispersion with longitudinal dispersion length equal to 0.1 m. In a fully saturated constant velocity one-dimensional flow field, transport by Fickian longitudinal hydrodynamic dispersion is equivalent to molecular diffusion. From Eq. 5, we see that a Darcy velocity of 3.486e-7 m s^{-1} (pore velocity of 1.162e-6 m s^{-1}, or 0.1 m/day at 30% porosity) and longitudinal dispersivity of 0.1 m corresponds to a dispersion coefficient of 3.486e-8 m^2 s^{-1}. Using the same porosity and assuming tortuosity of 1.0, the equivalent molecular diffusivity is 1.162e-7 m^2 s^{-1}. Thus identical results will be obtained using EOS7R and molecular diffusivity equal to 1.162e-7 m^2 s^{-1} as with T2DMR with longitudinal dispersion coefficient equal to 3.486e-8 m^2 s^{-1}. The input file shown in Fig. 3 includes a diffusivity of 1.162e-7 m^2 s^{-1} and is for running without the dispersion module. The mesh file for this one-dimensional flow problem is 2 grid blocks wide in the Z-direction to conform to requirements of the dispersion module and facilitate intercomparison between EOS7R and T2DMR. An analytical solution for this problem is given in Javandel et al. (1984). The numerical solution is accomplished by specifying constant pressure boundary conditions which will give rise to a steady-state flow field with pore velocity equal to approximately 0.1 m/day.

```
*SAMR1*  1-D RADIONUCLIDE TRANSPORT (NO GRAVITY)

         Note new parameters XKD3 and XKD4 in 'ROCKS' block.  XKD3 is
         set to 1.62e-04 which gives rise to a retardation factor of 2
         for this single-phase flow problem with porosity of .30.
         Note tortuosity is set equal to 1.0.

ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
FINE     2     2650.       .30  1.24E-09  1.24E-09  1.24E-09       1.8     1030.
                                      1.            1.62e-04  0.00E-00

    1            0.        0.        1.        1.
    1          0.e6        0.        1.

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

         MOP(19) = 0, INCON is in EOS7R format.
         MOP(19) = 1, INCON is in EOS7 format.

PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3 121     1211     00  0031 40 0
            1.728e6       -1.      2.e4             0.00000
    3.e+01
    1.E-05      1.E0
           1.0000E5                 0.0                 0.0                 0.0
                25.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    4    4    2   10
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1
   1.728e6

         Records 1 and 4 in 'SELEC' block include parameters needed
         by the dispersion module only.

           1. IE(1),NGBINP(1),NGBINP(2),NGBINP(3)
              Read in number of records (6) of dispersion and
              radionuclide data, and the number of gridblocks in the
              X-, Y-, and Z-directions.  The parameters NGBINP(1,2,3)
              are needed only for the dispersion module, T2DM.

           4. ALPHAT, ALPHAL
              Transversal and longitudinal dispersivities.  Used
              only by T2DMR.

         Records 6 and 7 in 'SELEC' block specify radionuclide
         parameters.

           6. XHALF(3),XMW(3),FDDIAG(NP,NK),(NK=3,NP=1,2),HCRN1
              Read half-life, in s, molecular weight, diffusivities,
              and the inverse Henry's Constant for radionuclide
              component 1, the parent.  Note for this single-phase
              problem, the volatilization has been neglected by
              setting the inverse Henry's Constant very large.

           7. XHALF(4),XMW(4),FDDIAG(NP,NK),(NK=4,NP=1,2),HCRN2
              Read half-life, in s, molecular weight, diffusivities,
              and the inverse Henry's Constant for radionuclide
              component 2, the daughter.  Note for this single-phase
              problem, the volatilization has been neglected by
              setting the inverse Henry's Constant very large.


SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6    1   24    2
     -1.e5

     0.e-0     0.e-1
     0.e-6     0.e-6     0.e-6  1.162e-7     0.e-6     0.e-6
  1.728e06     234.0     0.e-6  1.162e-7                         1.e+30
   1.00e40     230.0     0.e-6  1.162e-7                         1.e+30

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1
          100001.75                  .0                0.01                 0.0
                25.
A21 1
          100001.75                  .0                0.01                 0.0
                25.
A1O 1
               1.E5                  .0                 0.0                 0.0
                25.
A2O 1
               1.E5                  .0                 0.0                 0.0
                25.

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

ENDCY
MESHM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

XYZ
        0.
NX       1        1.
NY       1     1.e-6
NY       1     .1250
NY      12       .25
NY       2     .3125
NY       6       .50
NY       1       .25
NY       1     1.e-6
NZ       2        1.
ENDFI
```

Fig. 3. Input file for one-dimensional radionuclide transport.

The MESH files were created with MESHMAKER and then edited "by hand" to give the left- and right-hand side columns of grid blocks volumes larger than 1.e50 m^3 so that their pressures and component mass fractions remain effectively constant. We specified initial conditions such that the pressure difference between the left and right sides gives rise to a pore velocity of 1.162e-6 m s^{-1} (≈ 0.1 m/day). The concentration of parent radionuclide (RN1) is set to 1.e-2 in the left-hand side (grid blocks A11 1 and A21 1). These initial conditions are shown in the INCON block of the input file in Fig. 3. Note that by making the reference pressure negative, the brine is made a tracer chemical component with identical thermophysical properties as pure water. It should be pointed out that the radionuclide concentration could be considered either a mass fraction or a mole fraction since this concentration will have no effect whatsoever on the transport properties of the liquid. Furthermore, since only the decay of the parent is being considered, the ratio of molecular weights does not enter the equations and we have arbitrarily set the molecular weight of the decaying component to 234 g/mole.

We present results from simulations using a coarse (24 x 2 grid blocks) and a fine (112 x 2 grid blocks) spatial discretization. Concentration profiles for the transport of radionuclide 1 (RN1, the parent) at t = 20 days are shown in Figs. 4 and 5, for the coarse and fine grids, respectively. The analytical solutions calculated after Javandel et al. (1984) are shown by the lines. Four different cases are plotted: (1) no decay (half-life of RN1 is infinite, no adsorption (R = 1); (2) half-life of RN1 is 20 days, R = 1; (3) half-life of RN1 is 20 days, R = 2; and (4) no decay, R = 2. The plotted symbols are at the nodal points and show mass fraction (X). Results for the two different discretizations show the expected trend toward diminished numerical dispersion and improved agreement with the analytical solution as the spatial discretization is made finer. The time-step size was held to a maximum of 2.e4 seconds for both the fine and the coarse discretizations. Note that this maximum time step is approximately 1/100 of the shorter half-life.

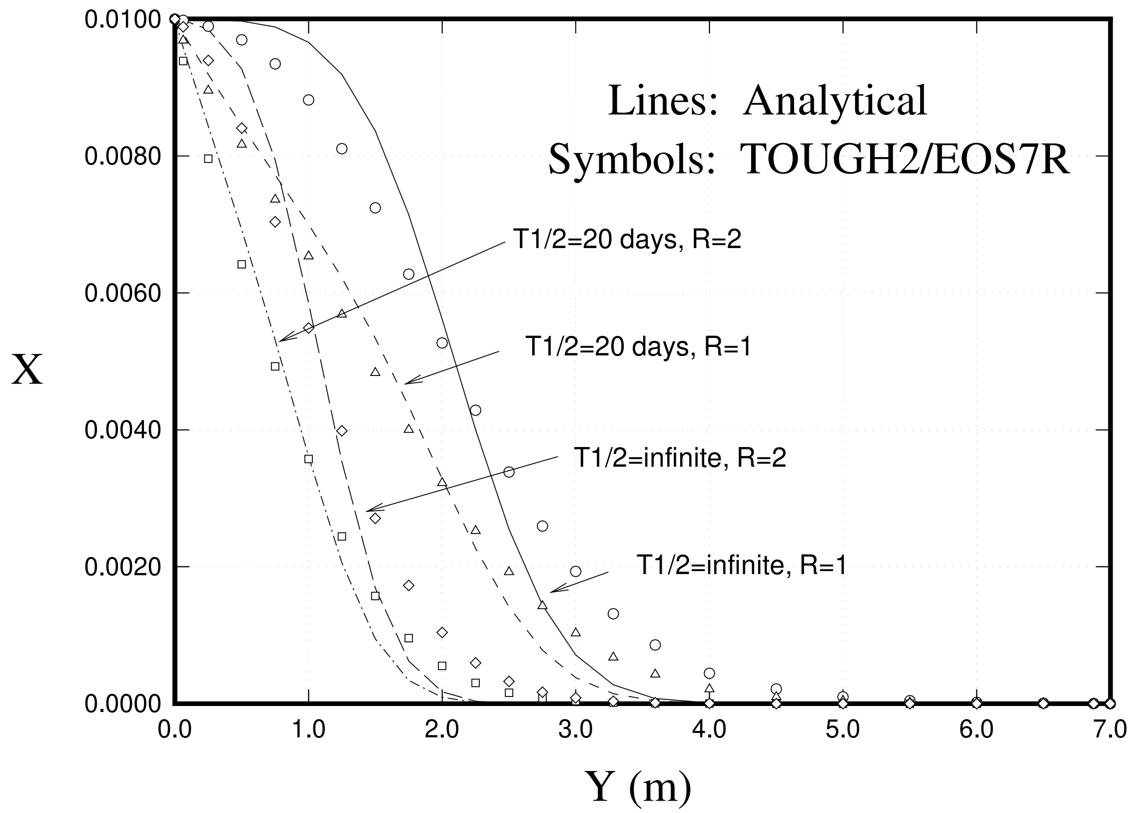

Fig. 4. Parent radionuclide mass fraction after 20 days for the coarse grid (24 x 2). Symbols show numerical result, lines are analytical solution.

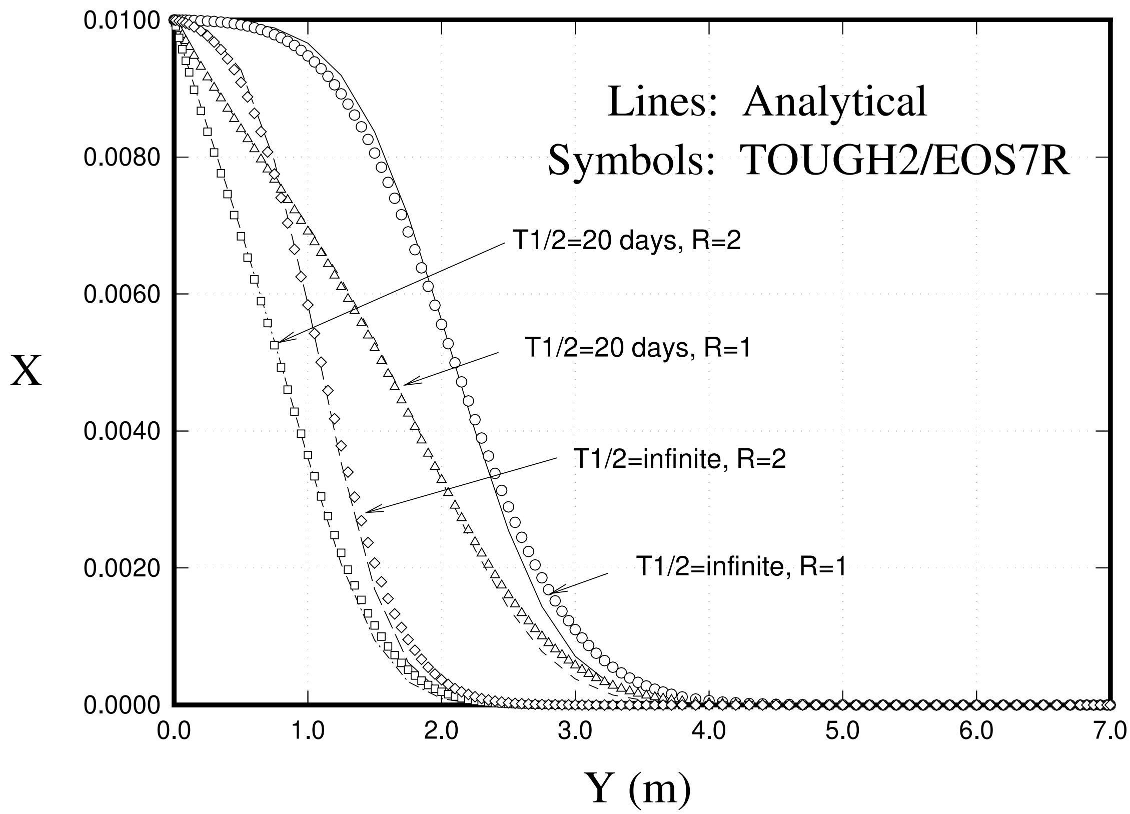

Fig. 5. Parent radionuclide mass fraction after 20 days for the fine grid (112 x 2). Symbols show numerical result, lines are analytical solution.

The second variation of the problem considers two-phase flow. In the problem, two-phase conditions are prescribed on the left-hand side of the domain. The inverse Henry's constants (solubilities) for the parent and daughter are set to the relatively small value of 1.0e-6 Pa^{-1} so that parent and daughter partition into the gas phase. Molecular diffusivities for air, parent, and daughter components have also been made non-zero for the gas phase. The input file for this variation is shown in Fig. 6. Coarse grid (24 x 2) results showing concentration of parent and daughter in the gas phase are presented in Fig. 7.

```
SAMR1*  1-D RADIONUCLIDE TRANSPORT (NO GRAVITY)

         This input file is for a two-phase variation of samr1.
         Note the relative permeability and capillary pressure functions.

ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
FINE     2     2650.       .30  1.24E-09  1.24E-09  1.24E-09       1.8     1030.
                                      1.            1.62e-04  0.00E-00

    1            .2        0.        1.        1.
    1          0.e6        0.        1.

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

         MOP(19) = 0, INCON is in EOS7R format.
         MOP(19) = 1, INCON is in EOS7 format.

PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3 121     1211     00  0031 40 0
          1.728e6       -1.      2.e4             0.00000
    3.e+01
    1.E-05      1.E0
            1.0000E5                0.0                 0.0                 0.0
               10.6                 25.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    5    5    2   11
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1
   1.728e6
              Note in SELEC.6 and SELEC.7 the value of the inverse
              Henry's Constant is set to 1.e-06 which will make
              both parent and daughter partition into the gas phase.

SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6    1   24    2
     -1.e5

     0.e-0     0.e-1
     0.e-6     0.e-6     1.e-5  1.162e-7     0.e-6     0.e-6
  1.728e06     234.0     1.e-5  1.162e-7                         1.e-06
   1.00e40     230.0     1.e-5  1.162e-7                         1.e-06

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1
           100001.75                 .0                0.01                 0.0
                10.6                25.
A21 1
           100001.75                 .0                0.01                 0.0
                10.6                25.
A1O 1
                1.E5                 .0                 0.0                 0.0
                10.6                25.
A2O 1
                1.E5                 .0                 0.0                 0.0
                10.6                25.

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

ENDCY
MESHM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

XYZ
        0.
NX       1        1.
NY       1     1.e-6
NY       1     .1250
NY      12       .25
NY       2     .3125
NY       6       .50
NY       1       .25
NY       1     1.e-6
NZ       2        1.


ENDFI
```

Fig. 6 Input file for the two-phase variation of SAMR1.

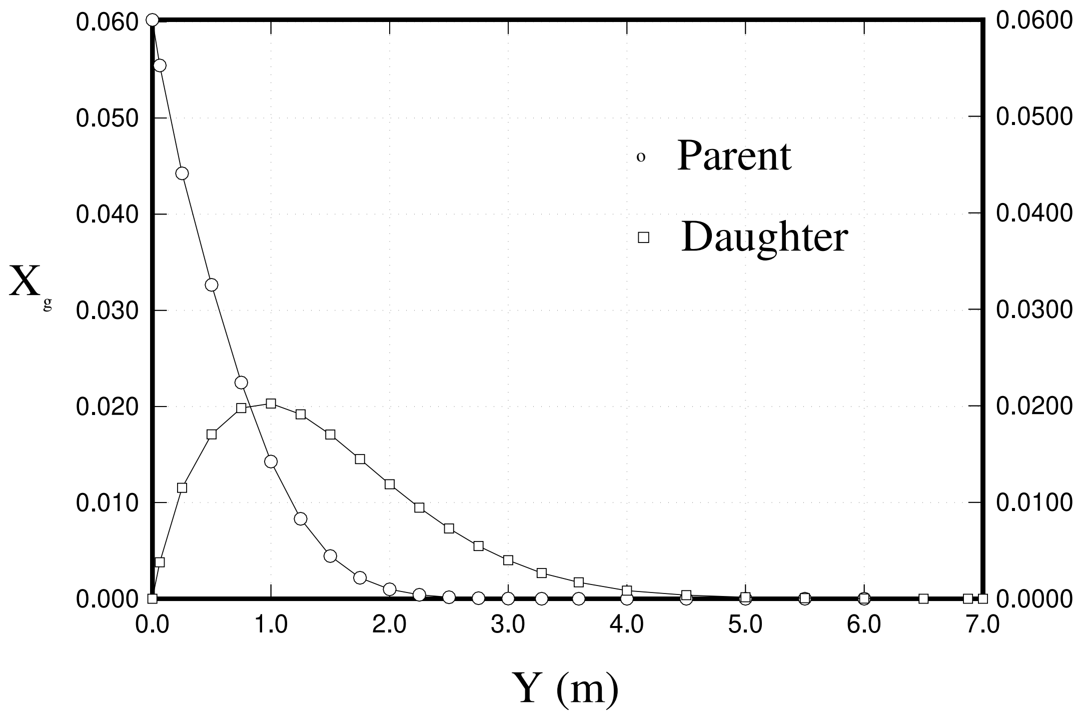

Fig. 7. Parent and daughter mass fractions in the gas phase after 20 days for the two-phase variation of SAMR1.

5.2. *One-Dimensional Transport and Decay of Ammonium*

In this problem, we compare results from EOS7R with analytical solutions for the problem of the microbially mediated first-order oxidation of ammonium ("parent") to nitrite ("daughter"), and the subsequent oxidation of nitrite. This problem was considered first by Cho (1971) and subsequently by vanGenuchten (1985) and McNab and Narasimhan (1993). The problem considers the flow of ammonium at a rate of 1 m/day pore velocity in a one-dimensional column 2 m in length. Two different discretizations were tested: (1) coarse, 102 grid blocks in the Y-dimension; and (2) fine, 402 grid blocks in the Y-dimension. Although the dispersion module is not used for this problem, the MESH was created with the needs of T2DMR in mind, thus NZ = 2 even for this one-dimensional problem. The half-lives of ammonium and nitrite used by Cho (1971) are 2.5e5 s and 2.5e4 s, respectively. The ammonium is adsorbed onto the solid grains with retardation factor $R = 2$; nitrite is not adsorbed. To achieve a retardation factor of 2 for the parent, we specify Kd = 9.43e-5 m^3 kg^{-1}; then from Eq. 16, we have R = 1. + (0.8 x 2650. x 9.43e-5)/0.2 = 2. The diffusion coefficient is d = 5.e-9 $m^2 \cdot s^{-1}$. Consistent with prior work (Cho, 1971; vanGenuchten, 1985; McNab and Narasimhan, 1993), we consider the concentration of decaying components to be in molar units. With this assumption, the ratio of molecular weights disappears from Eq. 25; we set the ratio equal to unity by assigning each molecular weight to that of ammonium (18 g/mole). Note that the choice of concentration units is arbitrary in this problem because the transport properties are entirely independent of the concentration of the decaying components. Although we formally use mass fractions for computing the solution with EOS7R, we present the results as if they were mole fractions to compare with the analytical solution. The input file for the problem is shown in Fig. 6. Note in the input file that the maximum delta-t (DELTMX of PARAM.2) is set to 2.5e3 s, or 1/10 of the smallest half-life. If the time-step size were allowed to grow to be comparable to or greater than the shortest half-life, severe time-discretization errors would arise.

The MESH files were created with MESHMAKER and then edited "by hand" to give the left- and right-hand side columns of grid blocks volumes larger than 1.e50 m^3 so that their pressures and component concentrations are effectively constant. We specified initial conditions such that ammonium is held in the left-hand side (grid blocks A11 1 and A21 1) at a concentration of 1.e-2 and the pressure difference between the left and right sides gives rise to a Darcy velocity of 5.56e-7 m s^{-1}. These initial conditions are shown in the INCON block of the input file in Fig. 8. Concentration profiles from EOS7R for ammonium (the parent) and nitrite (the daughter) are shown after 200 hours for the two grids in Figs. 9 and 10 along with analytical solutions. Note that we show only every fifth point with a symbol for the numerical solution. Agreement with analytical solution is good, with better results for the finer discretization.

```
*SAMR2*  1-D DECAY AND TRANSPORT OF CHO (Can. J. Soil Sci,51,339-350,1971).
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
FINE     2     2650.       .20  1.00E-12  1.00E-12  1.00E-12       1.8     1030.
                                      1.            9.43e-05  0.00E-00
    1           0.        0.        1.        1.
    1         1.e6        0.        1.

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3 301     3011     00  0031 40 0    0
             7.200e5       -1.    2.50e3             0.00000
    3.e+01
    1.E-05      1.E0
            1.0000E5                 0.0                 0.0                 0.0
                 25.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    4    4    2   10
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2
   3.60e05   7.200e5
SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6    1  102    2
     -1.e5

     0.e-0     0.e-0
     0.e-6     0.e-6     0.e-6  5.000e-9     0.e-6     0.e-6
   5.00e05      18.0     0.e-6  5.000e-9                        1.e+30
   2.50e04      18.0     0.e-6  5.000e-9                        1.e+30

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1
           100989.70                  .0                 .01                 0.0
                 25.
A21 1
           100989.70                  .0                 .01                 0.0
                 25.
C1W 1
                1.E5                  .0                 0.0                 0.0
                 25.
C2W 1
                1.E5                  .0                 0.0                 0.0
                 25.

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

MESHM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

XYZ
        0.
NX       1        1.
NY       1     1.e-6
NY     100     .0200
NY       1     1.e-6
NZ       2        1.


ENDFI
```

Fig. 8. Input file for one-dimensional transport and oxidation of ammonium.

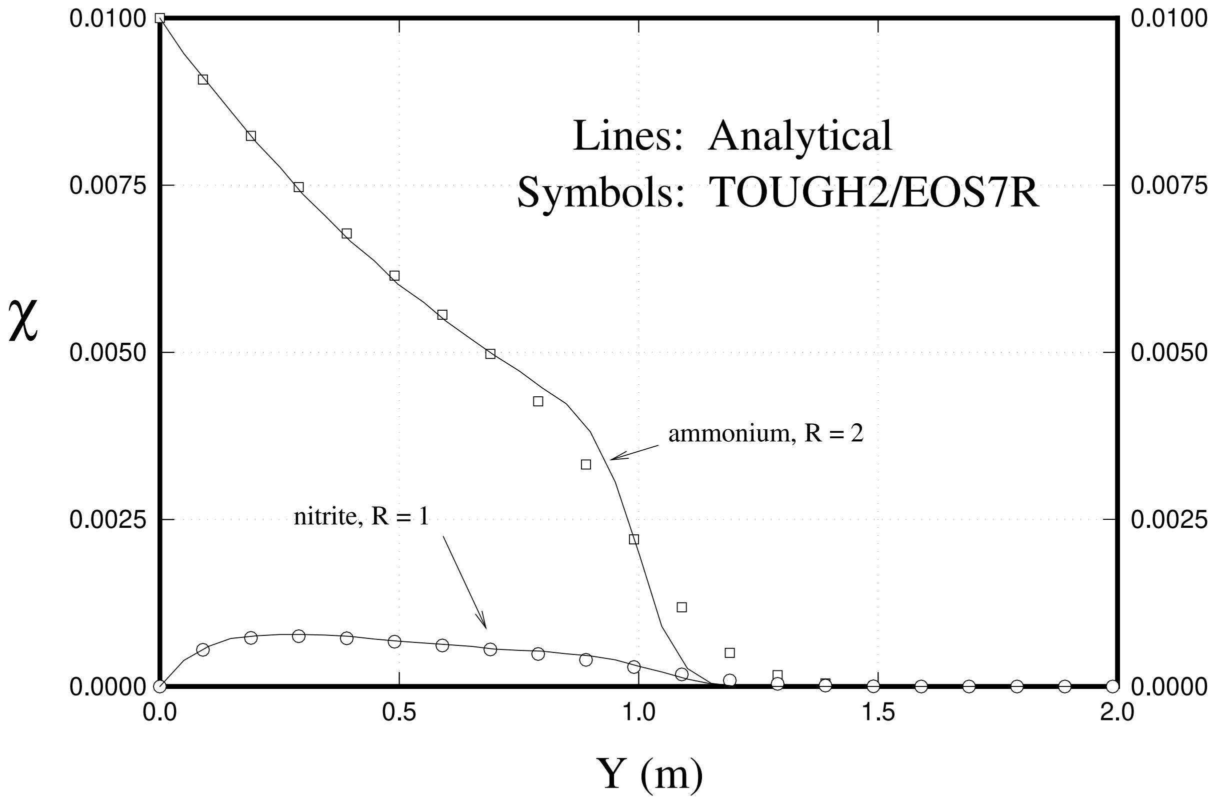

Fig. 9. Mole fraction profiles after 200 hours for the ammonium oxidation problem for the coarse grid (102 x 2 grid blocks). Symbols (every fifth point is shown) show numerical results while lines show analytical solution.

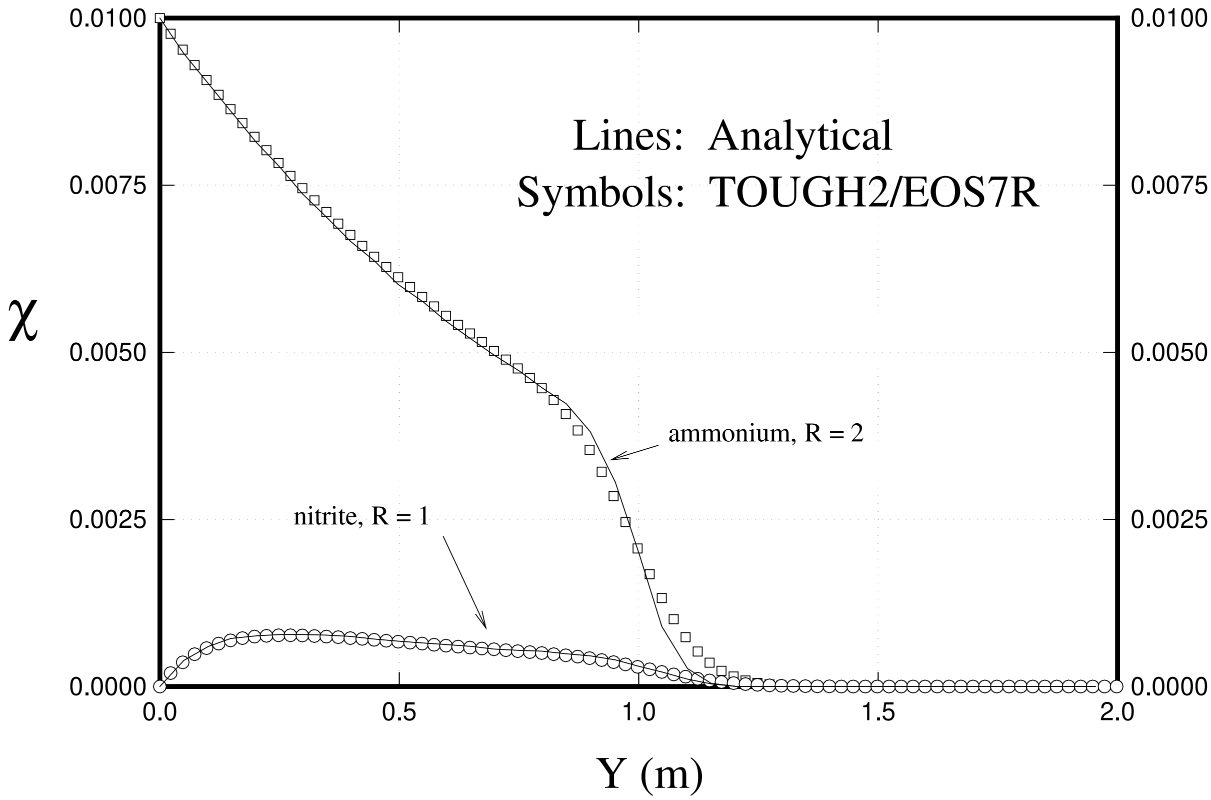

Fig. 10. Mole fraction profiles after 200 hours for the ammonium oxidation problem calculated on the fine grid (402 x 2 grid blocks). Symbols (every fifth point is shown) show numerical results while lines show analytical solution.

5.3 *Two-Dimensional Radionuclide Transport in a Salt-Dome Environment*

This problem considers the transport of hypothetical radionuclides in a steady-state flow field near a salt dome patterned after the conditions at Gorleben, Germany (Langer, et al., 1991; Oldenburg and Pruess, 1995). A schematic of the problem is shown in Fig. 11. The salt-dome flow problem involves large density changes due to salinity and is by itself a very challenging problem because of the strong coupling of the solute transport to the flow field. Because radionuclides are expected to act as trace components with negligible effects on liquid density, the radionuclide components do not affect the flow field. Thus, for this problem, we utilize the EOS7R capability of reading from a standard EOS7 INCON file consisting of the steady-state flow field calculated without consideration of radionuclide tracers. The method of solution is as follows. We first calculate the steady-state flow field for the salt-dome flow problem using T2DM as it is presented in Oldenburg and Pruess (1993, 1995). We then take the calculated steady state for brine and water alone and use it as the flow field for simulating the transport of radionuclides in the steady state. To do this, we use MOP(19) = 1 to read from the standard EOS7 INCON file which contains the steady-state results for the salt-dome flow problem. We then specify a constant generation rate of 1.6e-6 kg/s for component 3 (the parent, RN1) in the GENER block to model the leakage at a constant rate of radionuclide at a specific location. Alternatively, if one wanted to specify constant mass fraction in a grid block, one could read from the EOS7 INCON file (MOP(19) = 1), go forward one very small time step (say, 1.e-9 seconds), and edit the SAVE file to specify the desired mass fraction of radionuclide in one grid block. Subsequently, this SAVE file is used as INCON, MOP(19) is set back to zero, and the radionuclide transport simulation is run using a MESH file with the appropriate volume for the radionuclide source grid block. If constant mass fraction of parent is desired, the source grid block volume must be set to a value larger than 1.e50 m^3. For decaying parent in the source grid block, the volume should be made smaller than 1.e50 m^3.

We inject parent radionuclide into a region of 30 m x 15 m = 450 m^2, centered at Y = 150 m, Z = -232.5 m (Fig. 9). The half-life for the parent radionuclide is chosen as $T_{1/2}$ = 50 years, and the half-life of the daughter is 250 years. The flow field and concentrations for the parent and daughter radionuclides after t = 20, 60, 100, and 1400 years are shown in Figs. 12 and 13. The travel time across the domain is about 50 years. In Fig. 12, we see the parent transported downstream and undergoing decay such that it is in approximate steady state by t = 100 years. In Fig. 13 we see the interesting result that the maximum daughter concentration at t = 1400 years does not occur downstream from the parent source, but instead occurs in the weak recirculation region. A more detailed analysis (Oldenburg and Pruess, 1996) reveals that parent enters the weak recirculation zone by transversal dispersion and resides there for a sufficiently long time so that significant amounts of daughter are produced. Once produced, the daughter cannot escape the weak recirculation; its half-life is long enough that it accumulates there as the parent decays.

Fig. 11. Variable density brine flow and dispersion problem. (a) Top pressure boundary condition. (b) Schematic of flow domain, with top and bottom boundary blocks shown filled by diagonal lines. (c) Flow domain discretization of 30 x 20 blocks with $\Delta Y = 30$ m and $\Delta Z = 15$ m. Shaded grid block indicates location of radionuclide injection. Grid blocks that are very small or outside the flow domain are not shown.

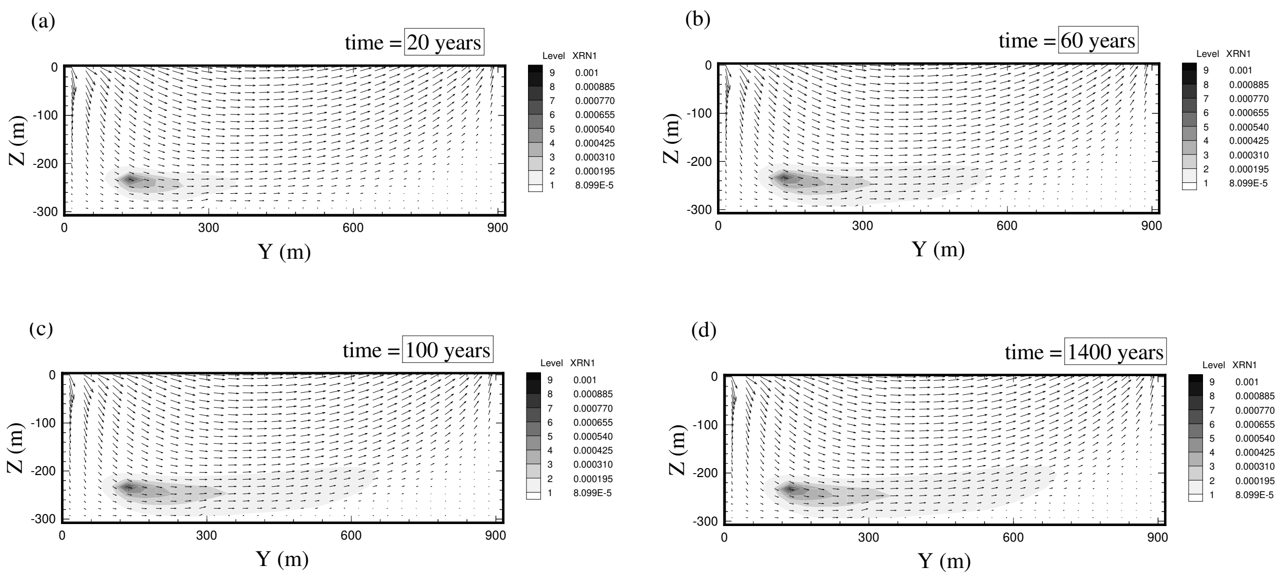

Fig. 12. Flow field and parent (RN1) radionuclide mass fractions at different times. Note the parent decays such that it is approximately at steady state after 100 years.

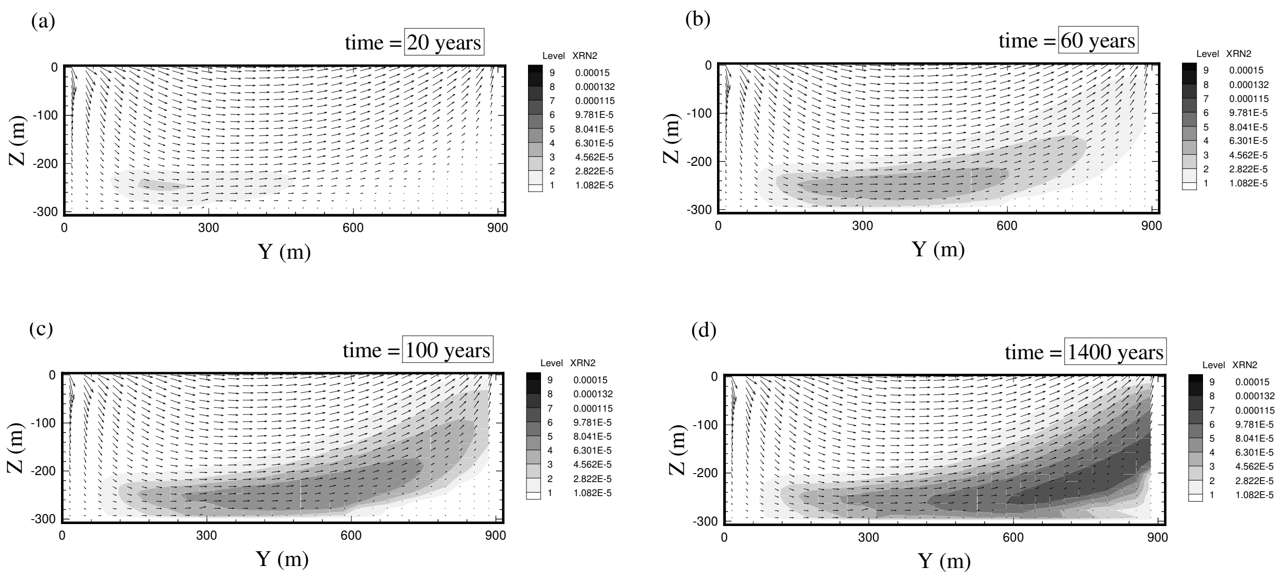

Fig. 13. Flow field and daughter radionuclide (RN2) mass fraction at different times. Note that maximum daughter concentration occurs in the weak recirculation zone in the lower right-hand corner of the domain.

5.4 *One-dimensional Volatile Tracer Transport*

In order to test and demonstrate the partitioning of tracer components between gas and aqueous phases, we examine the problem of downward transport of a stable volatilizing tracer for which an analytical solution has been presented by Shan and Stephens (1995). The current test problem considers the vadose zone transport by infiltrating water of an initial inventory of contaminant. The contaminant dissolves in the aqueous phase, volatilizes into the gas phase, and adsorbs onto the solid grains. The gas phase is immobile. Parameters for the problem are identical to those used in the problem of Fig. 6 in Shan and Stephens (1995) and are presented here in Table 3. The domain and boundary conditions are shown in Fig. 14.

Table 3. Parameters for the volatile tracer transport problem.

Parameter	Symbol	Value
porosity	ϕ	0.5
liquid saturation	S_l	0.1
permeability	k	1.030×10^{-12} m^2
pressure difference	ΔP	10.0 Pa
initial mass fraction	$X_{l,0}^{(\kappa)}$	1.0×10^{-4}
effective diffusivity (w)	$d_w^{(\kappa)}$	1.80×10^{-11} m^2 s^{-1}
effective diffusivity (g)	$d_g^{(\kappa)}$	5.88×10^{-7} m^2 s^{-1}
distribution coefficient	Kd	7.64×10^{-4} m^3 kg^{-1}
(Henry's constant)$^{-1}$	$1/H_{gl}^{(\kappa)}$	1.83×10^{-8} Pa^{-1}

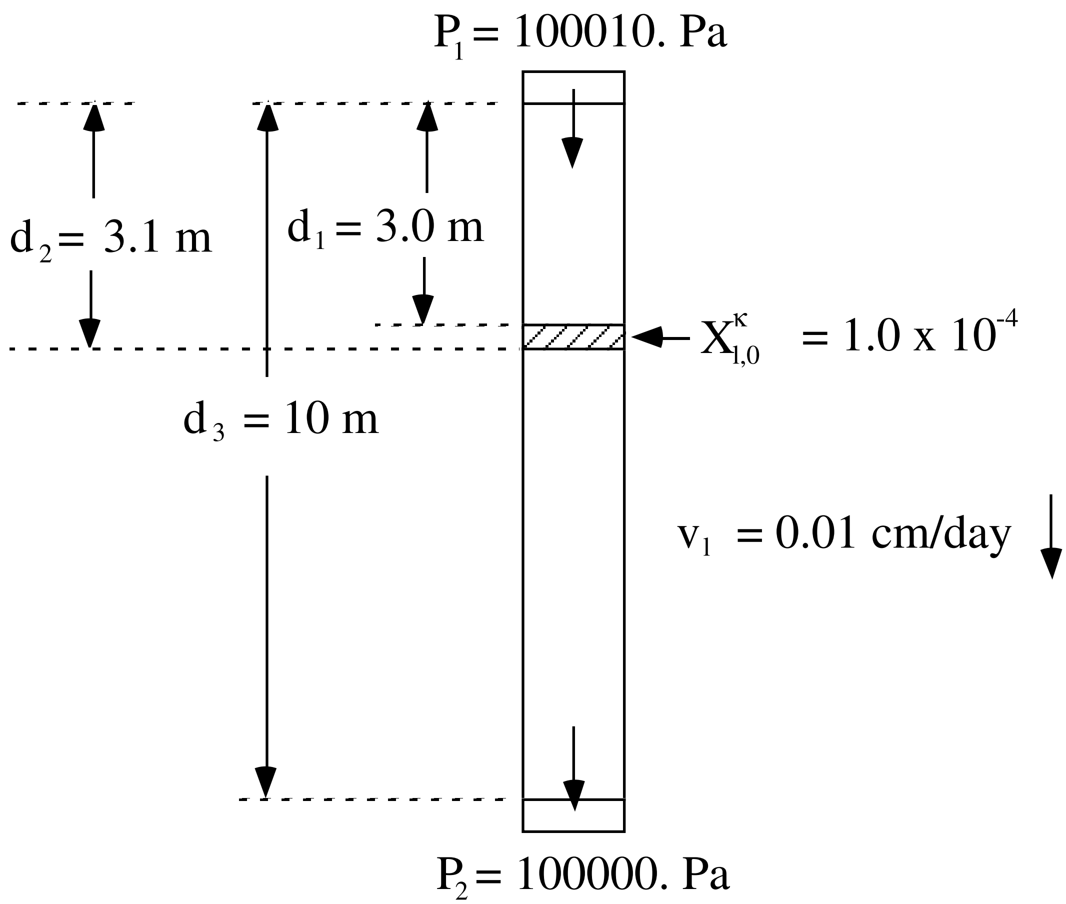

Figure 14. Domain and boundary conditions for volatile tracer transport problem. The initial mass fraction in the region .30 m < d < .31 m is 1.0×10^{-4}.

The domain was discretized into 100 grid blocks of 10 cm (0.10 m) each, with one boundary grid block on both the top and bottom for pressure and concentration boundary conditions. Fresh water enters at the top, while at the bottom the diffusive mass flux is specified as being zero. This boundary condition is implemented by specifying tortuosity (τ) of zero for the bottom gridblock. The EOS7R input file is presented in Fig. 15. Note that the molecular diffusivities are input as negative numbers and are equal to the effective diffusivities (Table 3) divided by porosity ($\phi = 0.5$). The negative value signals EOS7R to ignore phase saturation and material tortuosity (S and τ) for the calculation of diffusive fluxes. The division by ϕ was done to maintain the values shown in Table 3 for the calculation of diffusive fluxes in EOS7R where diffusivities are multiplied by ϕ. Results of the EOS7R solution and the analyical solution are shown in Fig. 16, where we plot the gas-phase concentration in the units used by Shan and Stephens (1995). Agreement is good. The smaller amount of diffusive smearing of the EOS7R solution relative to the analytical solution near the initial inventory arises because the numerical treatment cannot resolve the very large concentration gradient near the initial step-distribution leading to smaller diffusive flux away from the initial distribution. The initial inventory was discretized as one grid block. Note in the input file (Fig. 15) that major component diffusion is turned off, i.e., $d_w^{(H_2O)} = d_g^{(air)} = 0$. This was necessary to avoid multiphase effects where air would diffuse into the source grid block. As the relative permeability of gas in the source block is zero, this would lead to unphysical pressure buildup, the release of which can only occur by expulsion of aqueous phase from the source grid block.

```
*VOLAT*  1-D VOLATILE TRACER TRANSPORT
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
FINE     2     2300.       .50  1.03E-12  1.03E-12  1.03E-12       1.8     1030.
                                      1.                 7.64e-4
    1           0.        1.     1.e-9 1.0000001
    1         0.e6        0.        1.
TOP      2     2300.       .50  1.03E-12  1.03E-12  1.03E-12       1.8     2.e04
                                      1.
    1           0.        1.     1.e-9 1.0000001
    1         0.e6        0.        1.
BOT      2     2300.       .50  1.03E-12  1.03E-12  1.03E-12       1.8     2.e04
                                      0.
    1           0.        1.     1.e-9 1.0000001
    1         0.e6        0.        1.

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3 100     1001   0 00  0031 40 0                                  1.
          4.32e07       -1.                    0.00000
    3.e+01
    1.E-05      1.E0
           1.0000E5                .00                 0.0                 0.0
              10.60                25.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    5    5    2   11
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3
   8.640e6   2.592e7   4.320e7

SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6    1    1    1
     -1.e5

      0.e0      0.e0
-1.176e-06  0.00e-05  0.00e-05  0.00e-11  0.00e-11 -3.60e-11
  1.728e46      131.-1.176e-06 -3.60e-11                    1.83e-08
    1.0e40      233.-1.176e-06 -3.60e-11                     1.0e+51


INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1
          100010.00                 .0               0.e-6               0.e-7
              10.60                25.
AW1 1
          100000.00                 .0             7.40e-5               0.e-7
              10.60                25.

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

ENDCY
MESHM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

XYZ
        0.
NX       1        1.
NY       1        1.
NZ       1     1.e-5
NZ     100       .10
NZ       1     1.e-5


ENDFI
ENDCY



ENDFI
```

Fig. 15. Input file for the volatile tracer transport problem.

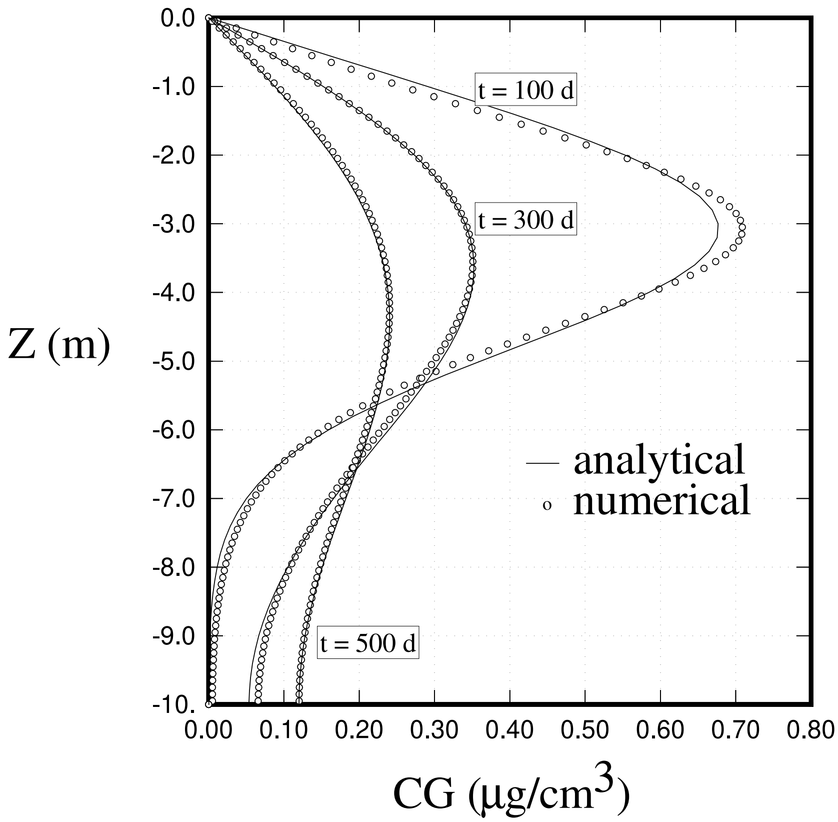

Fig. 16. Analytical and numerical (EOS7R) results at three different times for the volatile transport problem.

6. Final Notes

Summary of important points to remember in using EOS7R and T2DMR:

- EOS7R is an extension of EOS7 that includes parent and daughter radionuclide components and models diffusion, adsorption, and decay.
- T2DMR is a combination of EOS7R and T2DM. All of the information necessary for successful use of EOS7R and T2DM must be considered for successful use of T2DMR.
- MOP(19) selects the type of INCON file or block to be read from. For MOP(19) = 0, the INCON file is expected to be in the EOS7R format with up to 6 primary variables. For MOP(19) = 1, the INCON is expected to be in standard EOS7 format with up to 4 primary variables.
- The adsorption is specified by distribution coefficients *Kd* rather than by retardation factors *R*. Distribution coefficients may be specified separately for each domain by the new ROCK parameters XKD3 and XKD4.
- If a grid block volume is greater than or equal to 1.e50 m^3, the mass fractions of the radionuclide components will be held constant there. If the volume is less than 1.e50 m^3, then the mass fractions of the radionuclide components will change by first-order decay and production. This choice allows implementation of "constant concentration" as well as "fixed inventory" boundary conditions.
- EOS7R adds two components to EOS7 for a total of up to 6 components (NEQ = 6). Because the order of the Jacobian matrix is NEL x NEQ, users should expect execution times to increase significantly when radionuclide components are included. MOP(21) options allow selection of preconditioned conjugate gradient solvers for fast linear equation solution with execution times increasing approximately linearly with problem size.

- If molecular diffusivity is input as a negative number, the absolute value of this number is used for the phase molecular diffusivity without modification by S and τ (saturation and tortuosity) and without pressure or temperature effects. However, no diffusive fluxes are calculated for grid blocks where τ is input as zero or blank regardless of the phase molecular diffusivity.
- Pressure (*P*) affects gas diffusivity by the factor 1.e5/P (Pruess, 1987). For example, if pressure is 2.e5 Pa, the corresponding effective molecular diffusivity for the gas is one-half the input value.
- Temperature affects gas diffusivity by the factor $((T + 273.15)/273.15)^{TEXP}$ (Pruess, 1987)). If TEXP is input as zero, temperature effects on gas diffusivity are neglected.

Appendix 1. Program units in EOS7R.

MAIN
SUBROUTINE CYCIT
SUBROUTINE MULTI
SUBROUTINE OUTDF
SUBROUTINE INPUT
SUBROUTINE RFILE
SUBROUTINE INDATA
SUBROUTINE WRIFI
SUBROUTINE EOS
SUBROUTINE PP
SUBROUTINE VISCO
SUBROUTINE OUT
SUBROUTINE BALLA
SUBROUTINE QLOSS

Table A1. Summary of changes for program units in EOS7R.

Program unit	Basic changes for radionuclide transport
MAIN	Additional common blocks, changes in parameter statements to accommodate increased number of primary variables, new MOP options.
CYCIT	Changed to call OUTDF to printout dispersive fluxes.
MULTI	Added calculation of molecular diffusion for all components in all phases. Added calculation of first-order decay and adsorption for the parent and daughter components.
OUTDF	Changed to specify that fluxes are from diffusion only.
INPUT	Changed to accommodate increased number of primary variables. Added distribution coefficients as rock properties.
RFILE	Changed to read from standard EOS7 SAVE file.
INDATA	Changed to accommodate increased number of primary variables.
WRIFI	Changed to accommodate increased number of primary variables.
EOS	Changed to handle two additional volatile tracer components.
OUT	Changed to accommodate increased number of primary variables.
BALLA	Changed to accommodate increased number of primary variables.

Appendix 2. Program units in T2DMR.

MAIN
SUBROUTINE CYCIT
SUBROUTINE LINEQ
SUBROUTINE DISF
SUBROUTINE DOT
SUBROUTINE MESHM
SUBROUTINE GXYZ
SUBROUTINE OUTDF
SUBROUTINE SUMDUP
SUBROUTINE SUMDUP2

Table A2. Summary of changes for program units in T2DMR.

Program unit	Basic changes for calculating dispersive fluxes
MAIN	New common blocks, changes in parameter statements to accommodate increased number of primary variables and to account for 6 neighbor grid blocks used in calculation of dispersive fluxes, new MOP options.
CYCIT	Changed to call DISF to calculate dispersive fluxes, and SUMDUP to add duplicate entries in the Jacobian.
LINEQ	Changed to call DISF upon pivot failure.
DISF	Changed to neglect molecular diffusion if EOS7R was used.
DOT	No changes from T2DM.
MESHM	No changes from T2DM.
GXYZ	No changes from T2DM.
OUTDF	No changes from T2DM.
SUMDUP	No changes from T2DM.
SUMDUP2	No changes from T2DM.

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Nomenclature

d	molecular diffusivity	$m^2\ s^{-1}$
c	effective solute density	$kg\ m^{-3}$
CG	gas-phase concentration of Shan and Stephens (1995)	$\mu g\ cm^{-3}$
D	dispersion coefficient	$m^2\ s^{-1}$
$\overline{\mathbf{D}}$	dispersion tensor	$m^2\ s^{-1}$
f	adsorption ratio	–
$\mathbf{F}$	Darcy flux vector	$kg\ m^2\ s^{-1}$
$\mathbf{g}$	acceleration of gravity vector	$m\ s^{-2}$
$H_{gl}^{(\kappa)}$	Henry's constant	Pa
j	diffusive flux	$kg\ m^{-2}\ s^{-1}$
k	time-step index	
Kd	distribution coefficient	$m^3\ kg^{-1}$
M	mass accumulation term	$kg\ m^{-3}$
MW	molecular weight	$g\ mole^{-1}$

n	inward unit normal vector	
NEQ	number of equations per grid block	
NK	number of mass components (species)	
NPH	maximum number of phases present	
p	iteration index	
P	pressure	Pa
R	retardation	-
RN1,2	radionuclide 1 and 2	
q	source term	kg m^{-3} s^{-1}
S	phase saturation	-
t	time	days
$T_{1/2}$	half-life	s
v	coefficients of viscosity (see EOS7 report)	
u	magnitude of the Darcy velocity vector	m s^{-1}
u	Darcy velocity vector	m s^{-1}
V	volume	m^3
U	Y-component of Darcy velocity	m s^{-1}
X	mass fraction	-
Y	Y-coordinate	m
Z	Z-coordinate	m

Greek symbols

χ	mole fraction	-
Γ	surface area	m^2
λ	decay constant	s^{-1}
μ	dynamic viscosity	kg m^{-1} s^{-1}
ϕ	porosity	–
Φ	variable time-weighting parameter	

ρ	density	kg m^{-3}
τ	tortuosity	–

Subscripts and superscripts

a	air
g	gas phase
l	liquid
R	rock
w	aqueous phase
0	reference value
β	phase
κ	mass components