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Application of TOUGH2/EOS7R to Modeling of Radionuclide Release from a Low/Intermediate Level Repository under Two-Phase Conditions

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Abstract

The generation of gas due to corrosion of repository waste packages under water-saturated conditions will give rise to pressure increases and two-phase flow conditions. We have developed a numerical simulator TOUGH2/EOS7R for modeling the two-phase flow and transport of a parent-daughter pair of radionuclides including the processes of adsorption, first-order decay, binary diffusion, and volatilization. TOUGH2/EOS7R is a descendant of EOS7, the water, brine and air module of TOUGH2. We apply TOUGH2/EOS7R to an example problem relevant to the disposal of low- and intermediate-level nuclear wastes in crystalline rock. The conceptual model and spatial discretization were provided to us by NAGRA. We demonstrate in preliminary simulations that to good approximation, the generation of hydrogen can be modeled using air as a proxy for hydrogen. Simulations of gas generation and subsequent flow and transport away from the repository demonstrate the use and flexibility of TOUGH2/EOS7R. By small modification in the code, users can printout data for calculating the fractional release curve (FR curve), which shows the instantaneous release rate from the repository.

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1.0 Introduction

NAGRA (*Nationale Genossenschaft für die Lagerung radioactiver Abfälle*) is considering the disposal of low- and intermediate-level nuclear wastes in a geologic repository that would be situated in crystalline rock (Zuidema, 1994). Although matrix permeability of the host rock would be very low, fractures may be present which could conceivably provide pathways through which radionuclides could escape the repository and be released to the biosphere. Emplaced waste packages would be subject to corrosive attack from ambient groundwaters. Such corrosive processes are accompanied by the generation of hydrogen gas. Eventually the containers could be breached, and radionuclides could be released from the waste packages. Radionuclides could then migrate through the engineered barriers (backfill, liner) and fractures in the host rock by various transport mechanisms. Water-soluble radionuclides could be transported by advection and diffusion in ground water, while volatile radionuclides could be transferred into the gas phase and be transported by gaseous advection and diffusion processes. Transport processes could be strongly affected (retarded) by adsorption processes in backfill materials and host rocks.

In order to evaluate potential radionuclide releases, and assess the suitability of a proposed repository site, it is necessary to (a) develop a sound understanding of the hydrogeological conditions at the site, and (b) estimate the rates at which radionuclides could migrate along fractures and other permeable features that may be present.

We have developed a numerical simulator "TOUGH2/EOS7R" which provides a capability for mathematically modeling the important physical and chemical processes that affect radionuclide travel. A technical report is available that documents the processes described by the simulator, gives illustrative applications to a number of sample problems, and provides instructions for the preparation of input data (Oldenburg and Pruess, 1995). Briefly, TOUGH2/EOS7R can model the simultaneous flow and transport of five components, namely, (1) water, (2) brine, (3) parent radionuclide, (4) daughter radionuclide, and (5) air. The radionuclides may be volatile, i.e., they can (partially) be present in the gas phase, as well as being dissolved in the aqueous phase. They

may also adsorb on the rock. The air component in TOUGH2/EOS7R can represent, in an approximate way, the hydrogen that would be released during waste package corrosion.

The present report presents an example application of TOUGH2/EOS7R relevant to the disposal of low- and intermediate-level wastes. Our purpose is not to evaluate conditions and processes at any particular repository site. Accordingly, we are making liberal use of simplifying assumptions, such as a highly idealized geometry of the fracture-cavern system, homogeneous material properties in the various subdomains, and arbitrary properties for the tracer radionuclide components. The problem considered is patterned after earlier studies performed by NAGRA (Zuidema, 1994; Senger et al., 1994; Senger, 1995). It involves gas generation and radionuclide transport in a system consisting of a storage cavern, backfill, gas vent, liner, and a fracture in the host rock. The primary purpose of the report is to demonstrate the use of TOUGH2/EOS7R to the modeling of various multiphase transport processes in this type of system. It is hoped that the modeling approach and input data file presented here can serve as a template that will facilitate actual performance assessment studies.

The outline for this report is as follows. First, we discuss the lineage of TOUGH2/EOS7R and its relation to other members of the TOUGH2 family of codes. Then we present problem specifications and input files. The first simulation results we show are preliminary test cases that justify the use of air as a proxy for hydrogen. These are followed by presentation of the main simulation results. The final section summarizes the report.

2.0 Lineage of TOUGH2/EOS7R

TOUGH2/EOS7R is a descendant of EOS7 (Pruess, 1991b), the equation of state module for TOUGH2 (Pruess, 1991a) that handles water, brine, and air. With the addition of the variable density brine component in EOS7, TOUGH2 became capable of considering the flow of dense brines. We developed a code called T2DM (Oldenburg and Pruess, 1994) to provide the corresponding transport capabilities, specifically hydrodynamic dispersion and liquid-phase molecular diffusion. T2DM was developed for simulating variable density flow problems

associated with flow and transport in bedded salt formations. T2DM requires two-dimensional rectangular domains for calculating hydrodynamic dispersion. The interest of NAGRA in modeling two-phase transport of radionuclides prompted the current effort that produced EOS7R (Oldenburg and Pruess, 1995). TOUGH2/EOS7R adopted the molecular diffusion capabilities of T2DM, but does not include hydrodynamic dispersion. In this way, TOUGH2/EOS7R is not restricted to two-dimensional rectangular domains. When EOS7R is coupled with the dispersion module T2DM, one obtains T2DMR (see Oldenburg and Pruess, 1995) which can be used for modeling hydrodynamic dispersion of brine and volatile tracers with the restriction to two-dimensional rectangular domains. All of these modules handle isothermal and non-isothermal conditions. This history of code development is summarized in Table 1.

Table 1. Lineage of EOS7 modules.

	module	year	components	features
1	TOUGH2/EOS7	1991	water, brine, air	advective flow of water and dense brine mixtures.
2	T2DM/EOS7	1993	water, brine, air	As (1) with additional liquid-phase hydrodynamic dispersion and molecular diffusion restricted to 2-D rectangular domains.
3	TOUGH2/EOS7R	1995	water, brine, rn1, rn2, air	As (1) with additional volatile tracers, first-order decay chain, adsorption, and molecular diffusion.
4	T2DMR/EOS7R	1995	water, brine, rn1, rn2, air	As (3) with additional hydrodynamic dispersion restricted to 2-D rectangular domains.

3.0 Problem Specifications

3.1 Conceptual Model

The problem considers the corrosion of metals placed in a water-saturated cavern and the associated production of hydrogen gas. The production of gas in the saturated zone gives rise to the evolution of a gas phase with associated pressure buildup, and the subsequent flow of water and gas out of the repository through a vent at the top of the cavern. Radionuclides in the repository may then migrate by gas and aqueous phase advection and diffusion away from the repository and through fractures in the crystalline rock. The computational domain is a 150 m x 300 m two-dimensional cross-section of a cavern containing radioactive waste. This domain can be considered a planar fracture, or an axial cross section of a long cavern where the system is essentially two-dimensional. The cavern is excavated from crystalline rock, and includes an installed liner as well as backfill and waste. An elegant spatial discretization ("spider" mesh) was developed by NAGRA (Senger, 1994) and is shown in Fig. 1 with solid lines representing connections between grid blocks. The computational domain takes advantage of bi-lateral symmetry and models only the right-hand side of the system. The vertical coordinate is designated as the Y-coordinate in the spider mesh. Note that this domain violates the orthogonality assumption of the integral finite difference method, although we make no attempt here to evaluate errors associated with the use of this grid. In Fig. 2 we show a closeup of the cavern region with the various hydrogeologic units associated with the repository. Note that to model hydrodynamic dispersion with T2DMR, it would be necessary to use rectangular grid blocks (see Oldenburg and Pruess, 1993; 1995).

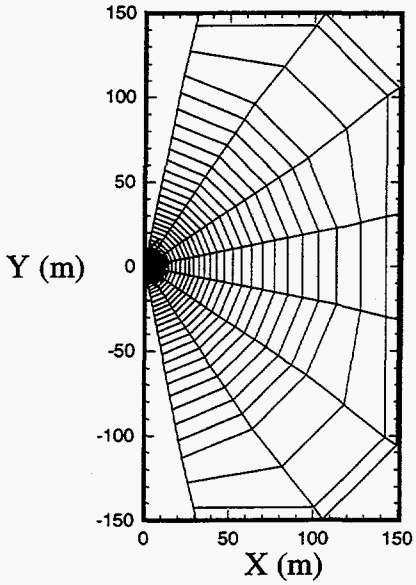

Fig. 1. One-half of the full cross-section domain showing spider mesh connections. Because of the symmetry about the Y-axis, only the right-hand side of the full domain is modeled.

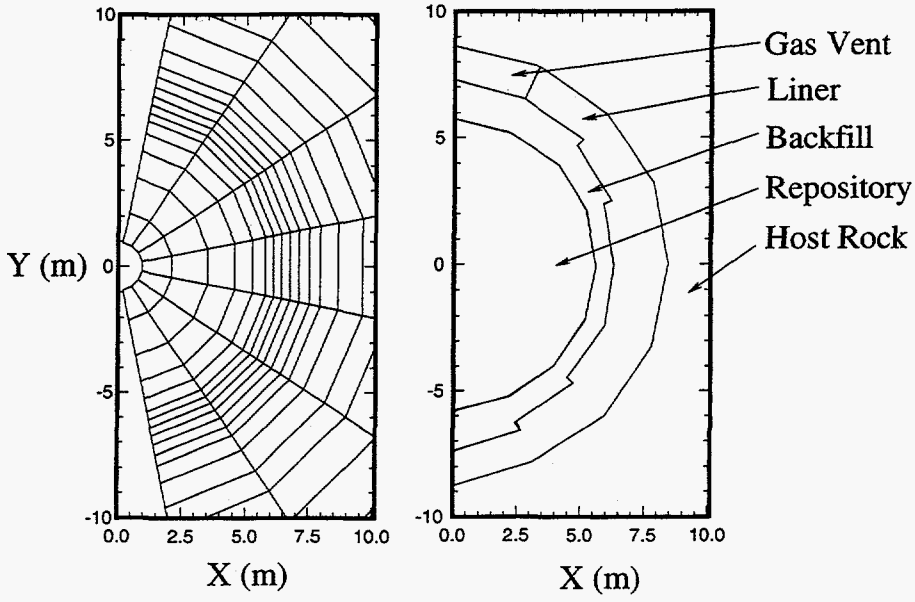

Fig. 2. Closeup of repository region showing spider mesh connections (left), and the domain boundaries for the gas vent, liner, backfill, repository, and a small portion of host rock (right).

Basic specifications for this problem were provided to us by NAGRA in the form of a TOUGH2 input file. These specifications with modifications and additions for EOS7R are shown in the input file of Fig. 3. Two new TOUGH2/EOS7R parameters in the ROCKS block are the distribution coefficients (Kd) for the two radionuclide components located in columns 51-60 and 61-70 of the second record of ROCKS parameters. Note that Kd for the parent component is zero and that Kd for the daughter component is 10 times smaller in the VMARL rock than in the other rocks to account for the fracture-dominated flow envisioned for the marl. Relative permeability is modeled with Corey curves with a residual gas saturation of .05, and we assume zero capillary pressure for the test problem. Note that the heat capacity of all materials other than the WASTE, BACKF, and LINER is larger than 1. x 10^4 J kg^{-1} $°C^{-1}$ so that mass balance is done only for these materials, facilitating the construction of the FR curve (see section 4.2). The original input file provided to us used very large material densities to ensure isothermal conditions. We have explicitly made the problem isothermal by specifying 5 equations and 5 components (NK = NEQ = 5) in the MULTI block. The GENER block has been changed to compensate for the larger molecular weight of air as compared to hydrogen. Space does not allow presentation of the ELEME, CONNE, or INCON blocks. The essential information in the ELEME and CONNE blocks is shown visually in Figs. 1 and 2. The latter (INCON block) can be summarized by stating that initial conditions are fully water-saturated, with hydrostatic pressure distribution throughout. The brine, parent and daughter mass fractions are 1.0 x 10^{-4} initially in the repository unit only. There is no air in the system initially. Boundary conditions are hydrostatic pressure and zero brine and radionuclide mass fractions on the bottom, top, and right-hand sides; the left-hand side (center line of complete system) is a no-flow boundary.

The SELEC block is where users specify the TOUGH2/EOS7R parameters such as molecular diffusivities, half-lives, molecular weights, and inverse Henry's constants. Values for the parameters for the test problem are shown in Table 2. The components designated as radionuclides are stable tracers (half-lives are 1. x 10^{40} and 1. x 10^{39} s). Because the purpose of this report is to demonstrate the use of TOUGH2/EOS7R in a general way and not to perform

analyses for any particular case, the properties for the radionuclide components correspond to arbitrary tracers and are not meant to represent any particular radionuclides.

Table 2. Parameters for the radionuclide components.

parameter	parent (rn1)	daughter (rn2)
distribution coefficient	0.	1. x 10^{-3}
half-life	1. x 10^{40} s (stable tracer)	1. x 10^{39} s (stable tracer)
molecular weight	246. gm $mole^{-1}$	246. gm $mole^{-1}$
molecular diffusivity	1. x 10^{-5} m^2 s^{-1} (gas) 1.x 10^{-9} m^2 s^{-1} (aqueous)	1. x 10^{-5} m^2 s^{-1} (gas) 1.x 10^{-9} m^2 s^{-1} (aqueous)
inverse Henry's constant	1. x 10^{-10} Pa^{-1}	2. x 10^{-10} Pa^{-1}
initial inventory	1.306 kg	5.225 kg

3.2 Tracer Modeling

Because the brine component can be modeled as a tracer component by specification of a negative reference pressure (see Pruess, 1991a), TOUGH2/EOS7R can actually consider three tracer components (brine, parent radionuclide [rn1], and daughter radionuclide [rn2]). If one gives each of these components different properties and behaviors, one can perform an experiment with three tracers in one TOUGH2/EOS7R simulation. For example, suppose we make brine a tracer component by giving it a negative reference pressure. The brine component does not adsorb nor volatilize. Thus it will be an aqueous phase tracer with no retardation, representing the worst-case aqueous phase transport scenario for a given molecular diffusivity. The parent component (rn1), can be assigned a small inverse Henry's constant such that it mostly volatilizes but does not adsorb. Thus the transport of rn1 will represent a worst-case gas-phase transport scenario. The daughter (rn2), can be made volatile and sorbing. Thus transport of the daughter will be retarded. We have assumed here that none of the components decays and they all have equal molecular diffusivities. Thus in one simulation, we can observe the behavior of three different tracer transport scenarios.

```
rq05kv3:  Gas Migration w/ liq. and gas tracers - Spider mesh: air.
ROCKS----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
WASTE    2     1.E03        .25    1.E-15    1.E-15    1.E-15       2.10    1000.
                                        1.        1.        0.       .001
    3              .25        .05
    1              0.         0.        1.
BACKF    2     1.E03        .25    1.E-13    1.E-13    1.E-13       2.10    1000.
                                        1.        1.        0.       .001
    3              .25        .05
    1              0.         0.        1.
LINER    2     1.E03        .20    1.E-19    1.E-19    1.E-19       2.10    1000.
                                        1.        1.        0.       .001
    3              .25        .05
    1              0.         0.        1.
AZON1    2     3.E03        .05    1.E-16    1.E-16    1.E-16       2.10     2.e4
                                        1.        1.        0.       .001
    3              .25        .05
    1              0.         0.        1.
AZON2    2     3.E03        .05    1.E-16    1.E-16    1.E-16       2.10     2.e4
                                        1.        1.        0.       .001
    3              .25        .05
    1              0.         0.        1.
AZON3    2     3.E03        .01    1.E-18    1.E-18    1.E-18       2.10     2.e4
                                        1.        1.        0.       .001
    3              .25        .05
    1              0.         0.        1.
VMARL    2     3.E03        .01    1.E-18    1.E-18    1.E-18       2.10     2.e4
                                        1.        1.        0.      .0001
    3              .25        .05
    1              0.         0.        1.
BOUND    2     3.E03        .01    1.E-18    1.E-18    1.E-18       2.10     2.e4
                                        1.        1.        0.         0.
    3              .25        .05
    1              0.         0.        1.
GVENT    2     1.E03        .30    1.E-13    1.E-13    1.E-13       2.10     2.e4
                                        1.        1.        0.         0.
    3              .25        .05
    1              0.         0.        1.

MULTI
    5    5    2   11
PARAM
 8 2 999     9991000001000000104000030000
     0.0E0 3.1536E10       -1.                              9.81
     1.E+2
     1.E-5
                2.5E6                    0.                1.e-5                  0.
                  0.                   10.

SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6
     -1.e5        25.      1200.
    1.e-30     1.e-30     1.e-30
       0.         0.
   1.0e-05   0.0e-05    1.0e-05   1.0e-09   1.0e-09   1.0e-09
   1.0e+40      246.    1.0e-05   1.0e-09                       1.00e-10
   1.0e+39      246.    1.0e-05   1.0e-09                       2.00e-10

TIMES
    3
  3.1536e7  3.1536e9 3.1536e10


GENER
    1T1       7    1    1    1     AIR   6.700E-09
    9T2       7    1    1    1     AIR   1.708E-08
   17T3       7    1    1    1     AIR   2.848E-08
   25T4       7    1    1    1     AIR   1.850E-08
   33T5       7    1    1    1     AIR   2.135E-08
```

Fig. 3. Selected parts of input file for the two-phase tracer transport problem.

3.3 Justifying the Use of Air as Proxy for Hydrogen

Corrosive processes in the repository will generate primarily hydrogen gas. As shown in Table 1, TOUGH2/EOS7R considers water, brine, parent, daughter, and air components. We show in this section that, to good approximation, air can be used as a proxy for hydrogen. In Table 3, we present some of the properties of hydrogen gas and air at 25 °C and 1 bar. We observe first in Table 3 that hydrogen is considerably less dense than air. At first this difference would seem to make dubious the use of air as a proxy for hydrogen. However, this problem is primarily a gas-liquid displacement problem. Thus the difference in density must be looked at in terms of the density difference between the gas and liquid phases. Although air is much heavier than hydrogen, when compared to water ($\rho = 997$ kg m^{-3}), both gases are very light. The difference in molecular weight is also large, but we can compensate for this difference by adjusting the mass generation rates of air to make the effective molar generation rates the same. The aqueous solubility values agree to within approximately 30%. In terms of the viscosities, we have approximately a factor of two difference.

Table 3. Selected properties of hydrogen and air at T = 25 °C and 1 bar.

	H_2	air	units
density	.0808	1.17	kg m^{-3}
MW	2.02	28.96	g $mole^{-1}$
aqueous solubility	1.91	1.38	cm^3 (100 g H_2O)$^{-1}$
viscosity	8.5×10^{-6}	1.8×10^{-5}	Pa s

Simulation results for the injection of hydrogen and air are presented here as evidence for the justification of the use of air as a proxy for hydrogen. The results are calculated using TOUGH2/EOS5 (for hydrogen) and TOUGH2/EOS7 (for air) with the adjustment that the mass generation rate of air is 14.34 times larger than the mass generation rate of hydrogen. This makes an approximately equal molar generation rate of air and hydrogen. Results after 100 yrs are presented in Fig. 4 in terms of gas saturation. Agreement is reasonable and appears to justify the use of air in place of hydrogen for this class of gas-liquid displacement problem. Further simulation results not presented here showed that gas-phase viscosity was the critical parameter controlling the differences in the hydrogen and air results for this problem.

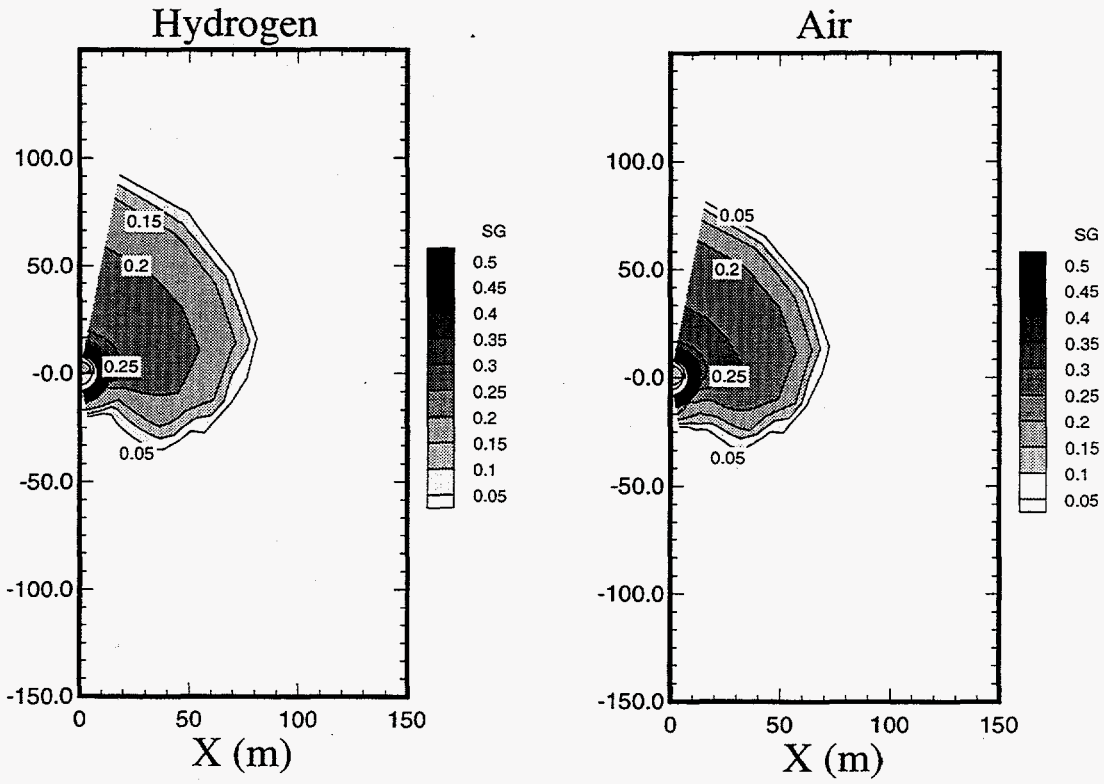

Fig. 4. Comparison of gas saturation for injection of hydrogen and air at equal molar injection rates.

4.0 Simulation Results

4.1 Early Time, t = 1 yr

Simulation results for the test case are presented in Figs. 5–9. We show results at t = 1 yr and t = 100 yrs for the liquid and gas phases and their dissolved components in turn. In Fig. 5 are shown the liquid saturation and logarithm (log) of the mass fractions of brine, parent, and daughter radionuclides in the aqueous phase at t = 1 yr for a region near the cavern. Superimposed on the contours are vectors showing the aqueous phase velocity; the largest vector corresponds to a phase velocity of 2.5×10^{-8} m s^{-1}. We observe at this early time the escape of water through the vent at the top of the cavern and the subsequent flow downward outside of the liner in the disturbed host rock around the cavern. Brine and parent (rn1) are distributed almost identically because at this early time the volatility and gas phase transport of the parent have not yet become important. The daughter (rn2) is already showing the effects of adsorption as its transport is retarded relative to the parent and the brine components. In Fig. 6 are shown the pressure, gas saturation, and log mass fractions of parent and daughter radionuclides in the gas phase at t = 1 yr for the same region immediately surrounding the cavern. Pressure buildup from the generated gas (air) causes the radial distribution observed near the cavern. This is a perturbation away from the initial hydrostatic pressure field. Gas saturations are low and confined to the respository at this early time as are the parent and daughter radionuclide components in the nascent gas phase.

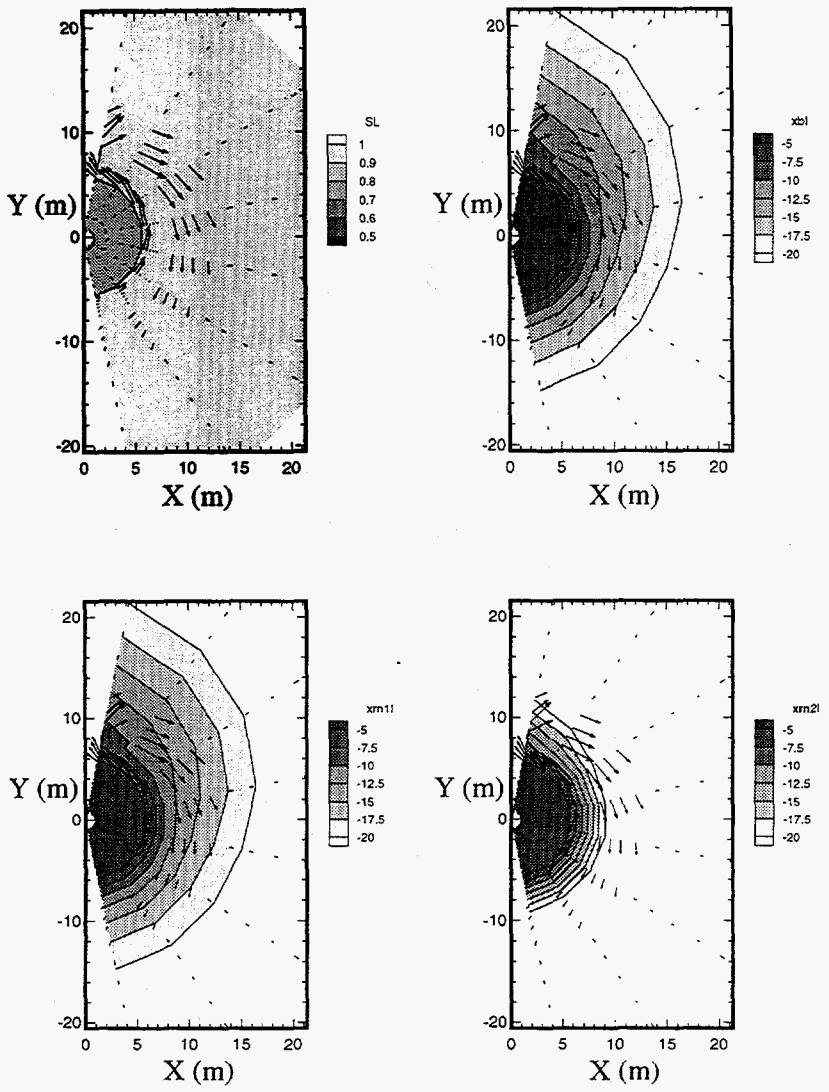

Fig. 5. Liquid saturation, and log mass fraction brine, parent (rn1), and daughter (rn2) in the liquid phase after 1 yr. Vectors show the aqueous phase velocity.

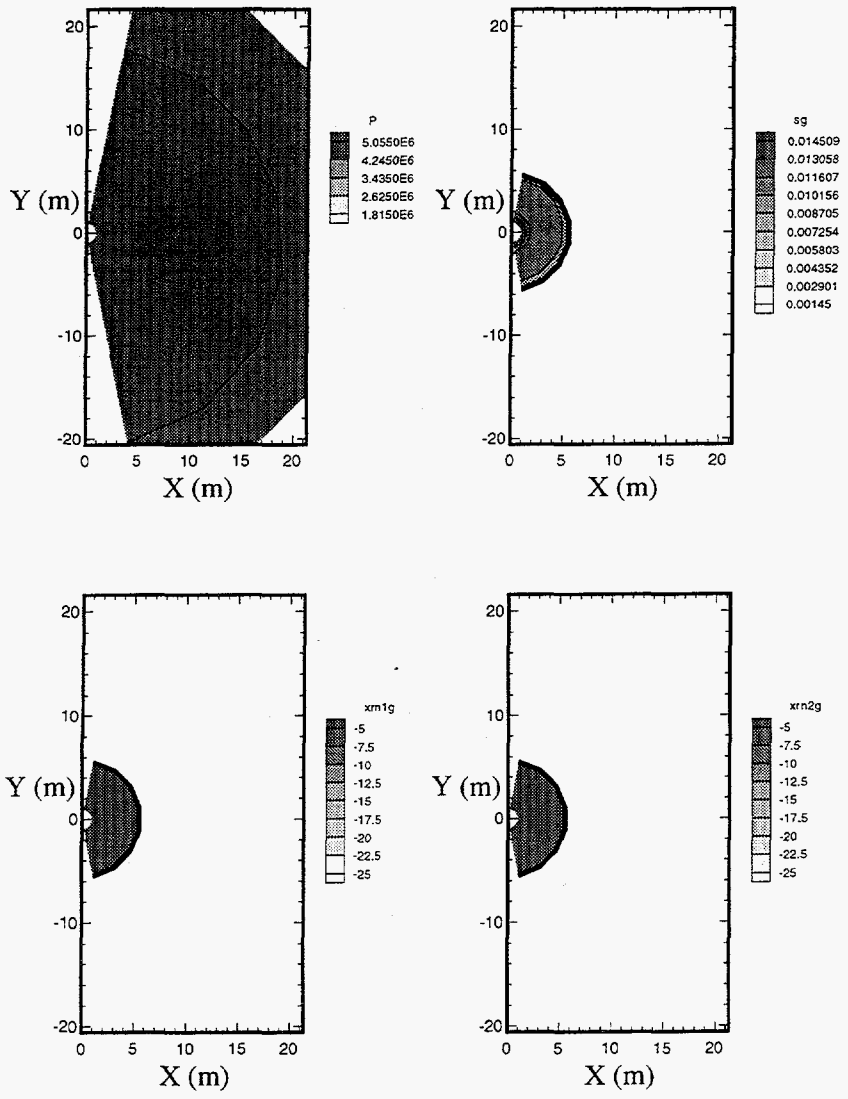

Fig. 6. Pressure, gas saturation, and log mass fractions of parent (rn1) and daughter (rn2) in the gas phase after 1 yr.

4.2 Later Time, t = 100 yrs

Results at t = 100 yrs are shown in Figs. 7–8 for the full domain. The very small vectors are aqueous phase velocity with the same scaling as in Fig. 5. Liquid saturation and logarithms of the mass fractions of brine, parent (rn1), and daughter (rn2) radionuclide components in the aqueous phase reflect the various properties of the different components at this time. Specifically in Fig. 7, we observe from the mass fractions that the volatile components (parent [rn1], and daughter [rn2]) generally move upward with the gas phase. The non-volatile brine tracer moves more radially outward and downward than upward near the repository where the aqueous phase is displaced by the produced gas. Note that the low concentration isopleths of brine mass fraction show the zero mass fraction brine boundary condition along the top boundary. This boundary effect can be avoided by setting the tortuosity of boundary grid blocks to zero to model a purely advective boundary condition with zero diffusive flux. Note the highest concentration of parent (rn1) in the aqueous phase is below the repository. The initial flux of water out of the top vent and around the disturbed zone coupled with the increased mixing and dilution around the top vent have led to this pattern. Retardation of the daughter (rn2) is evident by its more restricted distribution relative to the parent (rn1). In Fig. 8 are shown the pressure, gas saturation, and parent (rn1) and daughter (rn2) mass fractions in the gas phase at t = 100 years. The small vectors shown in places are for gas phase velocity, the largest vector representing a velocity of about 5. x 10^{-7} m s^{-1}. These results show the importance of gas generation. Namely, both radionuclides are transported away from the repository and generally upward. Retardation of the daughter (rn2) is apparent, but still allows 50 m of upward transport in 100 yrs.

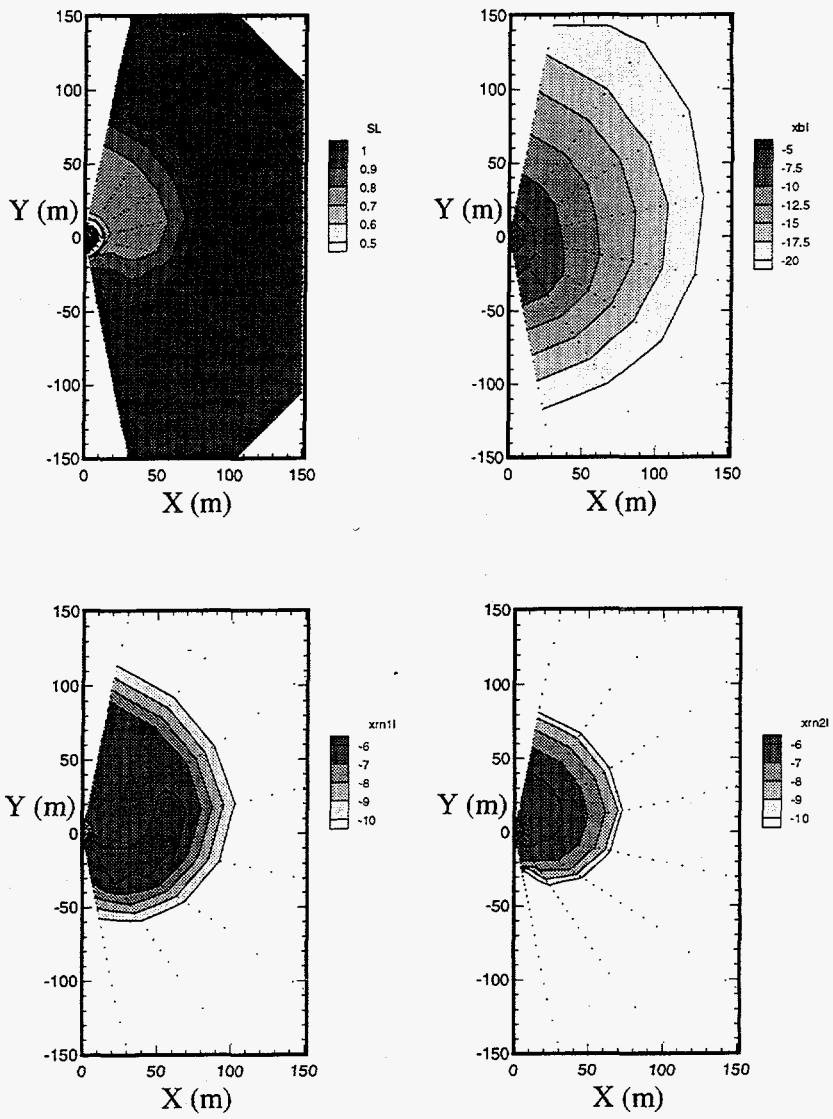

Fig. 7. Liquid saturation and log mass fraction of the brine, parent (rn1), and daughter (rn2) in the liquid phase after 100 yrs. The small vectors show aqueous phase velocity.

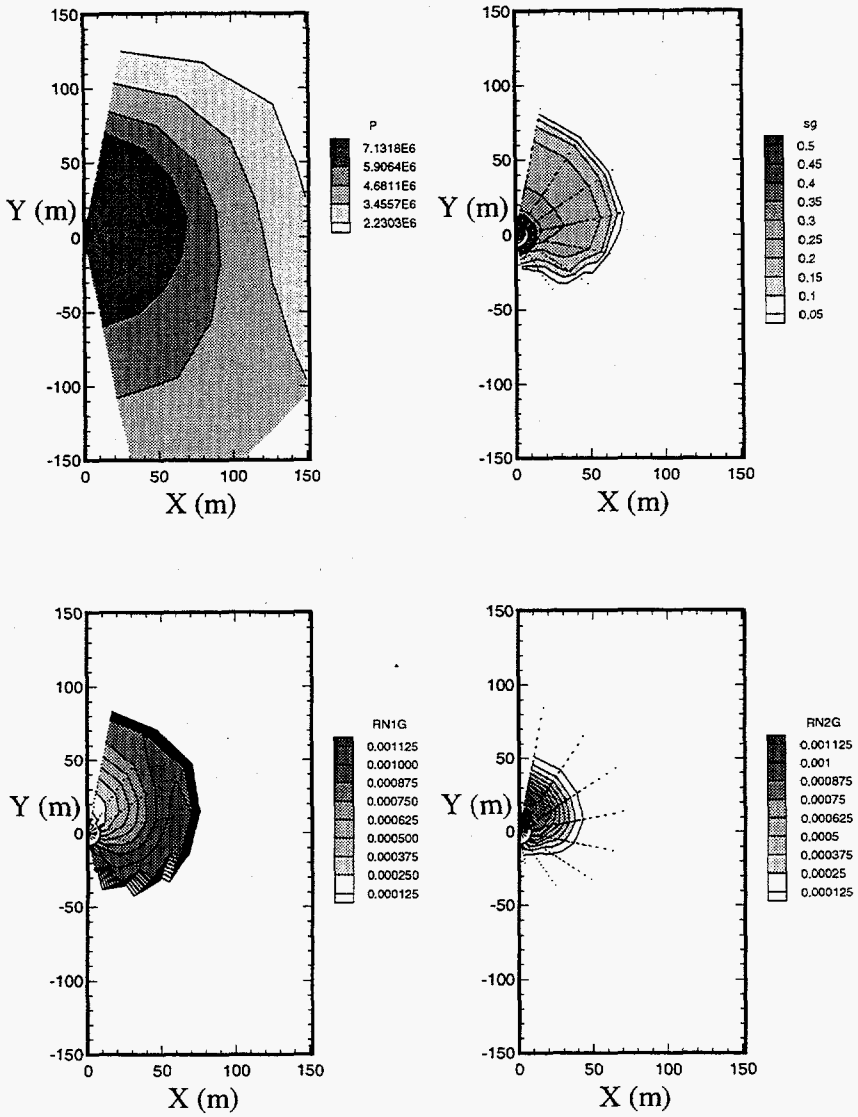

Fig. 8. Pressure, gas saturation, and mass fractions of parent (rn1) and daughter (rn2) in the gas phase after 100 yrs. The small vectors show gas phase velocity.

4.3 Fractional Release Curve

In prior work in liquid saturated conditions (Zuidema et al., 1994), the release of radionuclides from the repository has been quantified by defining an instantaneous release rate. This rate curve is called the fractional release curve, or FR curve, and can be defined identically for two-phase flow problems. The fractional release of a stable species κ is defined as

$$f_\kappa = \frac{M_\kappa(t) - M_\kappa(t+\Delta t)}{M_\kappa(0) \times \Delta t} \quad (1)$$

Here, $M_\kappa(t)$ is the inventory of κ at time t within the engineered barrier system (waste package, backfill, liner), $M_\kappa(0)$ is the initial inventory, and $M_\kappa(t) - M_\kappa(t+\Delta t)$ is the mass of species κ released to the host rock during a (short) time step Δt. The entire initial inventory $[M_\kappa(0)]$ of radionuclides is contained within the repository unit. However, by appropriate specification of heat capacities (see section 3.1), the mass at each time is calculated for the repository, backfill, and liner together. Thus the mass difference in the numerator is the mass lost from the repository, backfill, and liner over a time step Δt. In this way, the FR is a normalized instantaneous release rate, where release is defined as radionuclide passing beyond the liner.

The FR curve for the current test case is shown in Fig. 9. We observe in Fig. 9 small release rates initially. The difference in release rate is due to the different adsorption properties of the radionuclides. Specifically, a significant fraction of the daughter (rn2) is adsorbed and thus its transport is retarded. The sharp increase in release rate at about 7 years corresponds to the breakthrough of gas out of the gas vent. After 10 yrs, the release rate generally declines. Given the many approximations and assumptions in this example calculation, we caution readers that the FR curves shown cannot be taken to apply to actual radionuclide release.

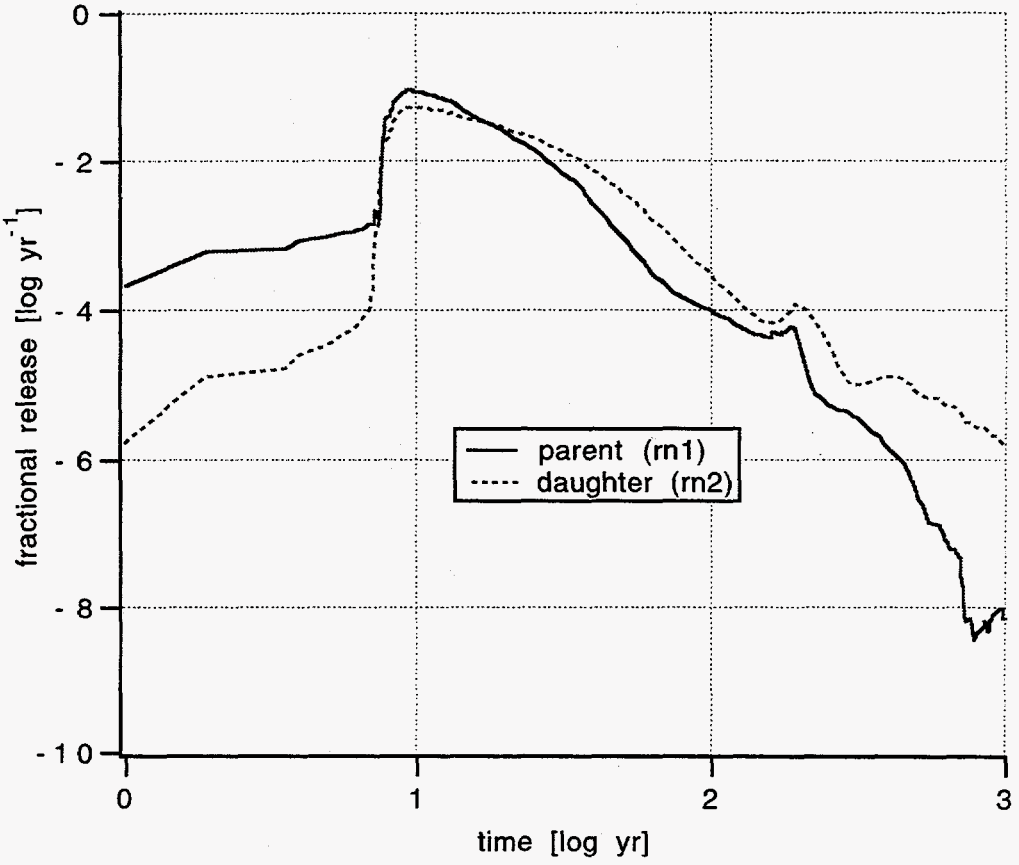

Fig. 9. FR curve for the parent (solid line) and daughter (dashed line). The daughter component is adsorbed on the matrix while the parent is not.

4.4 Obtaining Data for FR curve

Normally, subroutine BALLA for calculating summary mass and heat balances is only called for time steps at which printout is desired. To obtain data for calculation of the FR curve, users must uncomment the call to BALLA after every time step in subroutine CYCIT. While subroutine BALLA normally writes only to standard output, in TOUGH2/EOS7R, BALLA also writes to unit 50 (fort.50 on Unix operating systems). The file fort.50 contains three columns of numbers: (1) time [yr], (2) total mass of parent [kg], (3) total mass of daughter [kg]. Data in this file can then be used to produce the FR curve (Eq. 1) as a postprocessing step.

5.0 Conclusions

In this report, we have presented the application of TOUGH2/EOS7R to an example problem relevant to the transport of radionuclides in two-phase conditions. This simulation shows the importance of gas-phase transport in allowing radionuclides to migrate upwards with the buoyant gas. The flexibility in TOUGH2/EOS7R makes it possible to observe the behavior of a variety of tracers with different properties in a single simulation. A minor modification in the code will give printout for constructing fractional release (FR) curves. A complete description and users manual of TOUGH2/EOS7R is presented in Oldenburg and Pruess, 1995.

6.0 Acknowledgement

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7.0 Nomenclature

κ	component index
M	mass
rn1	Radionuclide 1, the parent
rn2	radionuclide 2, the daughter
t	time
X	mass fraction

8.0 References

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