Combined Gas and Nuclide Transport in a two dimensional Repository considering a variable Rock Convergence

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1   Introduction

To assess the long term safety of a repository for the radioactive waste in a deep salt rock formation, generally a brine inflow into the repository is postulated. The brine can react with the radioactive waste or with its containers and can gradually dis-assemble them. The radioactive substances after dissolved in brine can be transported out of the repository by rock convergence. The brine flow and nuclide transport can be enhanced by gas generation, mainly by hydrogen due to corrosion of containers and metallic materials. To analyse the combined impact of gas generation and rock convergence on nuclide transport, TOUGH2 is modified to simulate

–   variable rock convergence depending upon porosity and pressure,

–   permeability depending upon a variable porosity of a compactible filling material,

–   variable fluid flow induced by the rock convergence

in a two dimensional two phase system. Using these modifications in previous reports /JAV 96B, 96C/, combined gas and nuclide transport in a simplified two dimensional configuration consisting of a storage chamber, a drift and a shaft is studied assuming one drift level only. To extend these previous analyses, in the present paper, gas and nuclide transport in a repository with two drift levels is studied considering a hydrogen source influenced by the transient flooding of a repository, two phase flow, different filling materials, excavation disturbed zone, anisotropic diffusion and dispersion.

2   Modification of TOUGH2 Models

TOUGH2 assumes constant permeabilities and does not directly simulate the convergence of a salt rock. Hence, the calculation of a variable porosity n and permeability k of a compactible filling material is introduced considering a variable rock convergence depending upon pressure p and temperature T:

$$n = n(p, T, t) = V_{Void}/V_{total}, \quad n \geq n_{min}, \quad n_t = (1/n)(dn/dt) = C_L/n, \quad k = k(n),$$

$$C_L = C_{ref} f_1(p) f_2(n) f_3(T), \quad C_{ref} : \quad \text{Reference convergence rate of salt rock} = \text{constant},$$

$f_1 = (1 - p_F / p_{Rock})^m$, $n_1 = 1 - n / n_{Ref}$, $n_2 = (nn_1)^{(1/m)}$, $f_3 = 1$ for T = constant,

$f_2 = 1$ for $n \geq n_{Ref}$, $f_2 = nn_1 (n_1^2 + n_2)^{-m}$ for $n < n_{Ref}$, $C_L = 0$ for $n < n_{min}$.

The porosity change leads to an additional fluid flow Q, which is given by:

$S_F = V_F/V_{Void}$, $S_G = V_G/V_{Void}$, V_{total} = constant, $f_1 = 0$ if $p_F \geq p_{Rock}$,

$Q_{F,1,por} = |nV_{total} \, n_t \, \rho_F \, S_F \, X_1|$, $Q_{F,2,por} = |nV_{total} \, n_t \, \rho_F \, S_F \, X_2|$, $Q_{G,por} = |nV_{total} \, n_t \, \rho_G \, S_G|$.

Since the sophisticated dispersion model of /PRU 93/ assumes a fully two dimensional configuration, it is inexpedient to analyse a system, which consists of drifts and shafts mainly. Hence, a simplified model for dispersive flux G in liquid phase is introduced:

$D_{hor} = nd_{hor}$ (Domain) $S_F + \beta_{hor}$ (Domain) $|u|_{hor}$, $X_1 = m_1/m_F$, $X_2 = m_2/m_F$,

$D_{ver} = nd_{ver}$ (Domain) $S_F + \beta_{ver}$ (Domain) $|u|_{ver}$,

$(G_{1 \, or \, 2})_{hor} \sim D_{hor}$ [grad $(X_{1 \, or \, 2})]_{hor}$, $(G_{1 \, or \, 2})_{ver} \sim D_{ver}$ [grad $(X_{1 \, or \, 2})]_{ver}$.

The determination of flux G is similar to flux F in the dispersion model of /PRU 93/. However, this model modification does not assume a full two dimensional system as in /PRU 93/ and can easily be applied to a three dimensional configuration containing drifts and shafts. To implement all the modifications mentioned above, only three subroutines MULTI, QU and CONVER of the original version are extended.

3   Analysis

In the following two dimensional scoping analysis, a network of repository with two drift levels is postulated (Fig. 1). A storage chamber with radioactive materials in the left corner of the bottom drift at a depth of around 500 m is filled with compactible crushed salt and is connected to the shaft via two drifts. Both lower and upper drift are filled with a non compactible sealing material at the chamber side and with a non compactible filling material at the shaft side. Since the sealing material has a low permeability of $1 \cdot 10^{-17} \, m^2$, the excavation disturbed zone with the similar permeability along the drifts is also considered. Initialy, the repository is free from brine. The brine flows into the shaft and gradually into the chamber via two drifts. Simultaneously, the crushed salt is compacted by the variable rock convergence depending upon pressure and porosity in chamber. This reduces the void volume of the chamber. The radioactive substances (10^4 kg) in the chamber are simulated with a stable tracer in brine and can be driven out of the chamber by the pressurization due to gas production and by porosity reduction in chamber. The important parameters are /JAV 97B/:

–   Variable rock convergence and crushed salt properties: $C_{ref} = -5 \cdot 10^{-5}$ / year, $n_{Ref} = 0.3$, $n_{min} = 0.005$, $m = 4$, $p_{Rock} = 107$ bar, $k = (2 \cdot 10^{-9}) \, n^{4.5} \, m^2$.

–   Liquid phase : $\rho_F = \rho_{Tracer} = \rho_{Brine} = 1.292 \cdot \rho_{Water} (p, T)$; $\mu_F = 6.29 \cdot \mu_{Water} (p, T)$.

- Gas Phase (Hydrogen): gas constant = 4124 J / (kg·K), μ_G = 8.95·10⁻⁶ Pa sec.

- Brooks-Corey relations for two phase flow:

$$S_{F,eff} = (S_F - S_{Fr}) / (1 - S_{Gr} - S_{Fr}), \quad p_{cap} = p_{cap,min} / (S_{F,eff})^{0,5}, \quad S_{Gr} = 0.02; \quad S_{Fr} = 0.1;$$
$$k_{F,rel} = (S_{F,eff})^4, \quad k_{G,rel} = (1 - S_{F,eff})^2 (1 - S^2_{F,eff}), \quad k_F = k k_{F,rel}, \quad k_G = k k_{G,rel},$$

$p_{cap,min}$ = 1 bar for domain 8, 9, 12, 14 and 0 for domain 1, 11, 13.

In the first part of analysis, the brine inflow through the shaft without gas generation in chamber is studied with different reference convergence rates and p_{cap} = 0:

Case FL1: - 5 · 10⁻⁵ / year, **Case FL2:** - 5 · 10⁻⁴ / year, **Case FL3:** - 5 · 10⁻³ / year.

In the second part, a constant hydrogen generation rate in chamber is included from the time point, when S_F = 0.2 in chamber is reached, and its total generation depends upon the brine amount already present in the chamber at this time point. The hydrogen generation ends, when this brine amount is supposed to be utilised. To estimate the hydrogen generation depending upon inflow condition, the data of /JAV 97B/ for the same model are used: 133.6 kg/year consuming 5.97 · 10⁶ kg brine in 5000 years. In continuation of above inflow cases, three outflow cases are viewed assuming capillary pressure as defined above:

Case CT1: Initial chamber condition derived from the case FL1: S_F = 0.2, n = 0.191, m_F = 2.04 · 10⁶ kg at t = 9500 years; hydrogen generation 133.6 kg/year between 9500 and 11210 years, Δt_{Gen} = 11210 - 9500 = (2.04/5.97) (5000) years.

Case CT2: Initial chamber condition derived from the case FL2: S_F = 0.2, n = 0.0581, m_F = 6.29 · 10⁵ kg at t = 3900 years; hydrogen generation 133.6 kg/year between 3900 and 4427 years, Δt_{Gen} = 4427 - 3900 = (0.629/5.97) (5000) years.

Case CT3: Initial chamber condition derived from the case FL3: S_F = 0.2, n = 0.0113, m_F = 1.55 · 10⁵ kg at t = 1200 years; hydrogen generation 133.6 kg/year between 1200 and 1330 years, Δt_{Gen} = 1330 - 1200 = (0.155/5.97) (5000) years.

4   Results

These cases were computed with TOUGH2/EOS7 /PRU 91, 91A/ and variable rock convergence assuming three fluid components brine, tracer and hydrogen. The Fig. 2 and 3 show the liquid volume, void volume, liquid saturation and porosity in chamber during brine inflow situation. As expected, void volume and porosity are reduced rapidly with increasing rock convergence. The sealing material with k = 1 · 10⁻¹⁷ m² at the chamber entrance delays the brine inflow into chamber significantly. With increasing rock convergence, 20 % liquid saturation in chamber is achieved earlier (FL1: 9500, FL2: 3900 and FL3: 1200 years) and the flooding of the chamber ends faster (FL1: 22500, FL2: 7600, FL3: 2900 years). For further details, see the case NW1 in /JAV 97B/ which corresponds to present case FL1.

Fig. 4 to 6 reveal the chamber pressure, the gas and brine flow out of the chamber after the gas generation is initiated. With increasing rock convergence, the maximum chamber pressure is higher, because at the same constant gas generation rate the available void volume in chamber is smaller. But with decreasing rock convergence rate, the pressure peak duration is longer, since the gas generation period is longer. Such a high pressurization exceeding the lithostatic pressure can affect the mechanical stability of the filling or sealing material and repository substantially. The gas and liquid flow out of the chamber increases rapidly, as the chamber pressure due to gas generation rises, and decreases also rapidly as the gas generation ends. After that, the chamber pressure remains nearly constant at the hydrostatic level and the liquid flow is very low corresponding to porosity reduction in chamber due to rock convergence.

For an integral comparison, the nuclide removal from the chamber is depicted in Fig. 7. As expected, with increasing rock convergence the nuclide removal starts earlier. Though the mass flow out of the chamber is low in case CT3, the maximum nuclide removal is seen in case CT3 with the highest rock convergence. This occurs because the nuclide removal is mainly determined by the product $X_2 \cdot u_F$, which is considerably large due to small fluid volume in chamber in case CT3. In cases CT1 to CT3, the nuclide removal from the chamber is around 8 % within 15000 years. In case of no gas generation, there would be nearly no nuclide removal from the chamber within 20000 years, since the flooding of chamber would not be completed or liquid outflow would be negligible. In above cases, there is no nuclide removal at the top of the shaft, because the distance or the flow resistance between the chamber and the top of the shaft is relatively large. Further analyses including nuclide decay and adsorption are reported in /JAV 96C, 97B/. Summarizing, one can conclude from the scoping analyses, that the gas generation can enhance pressure build-up in storage chamber affecting the mechanical stability of the repository and nuclide removal substantially.

Symbols

d : molecular diffusivity [m^2/s]; k : permeability [m^2]; m : mass [kg]; t : time [s];
m : stress parameter; n : porosity; u : Darcy velocity; V : volume [m^3];
D : dispersion coefficient [m^2/s]; S : phase saturation; X : mass fraction;
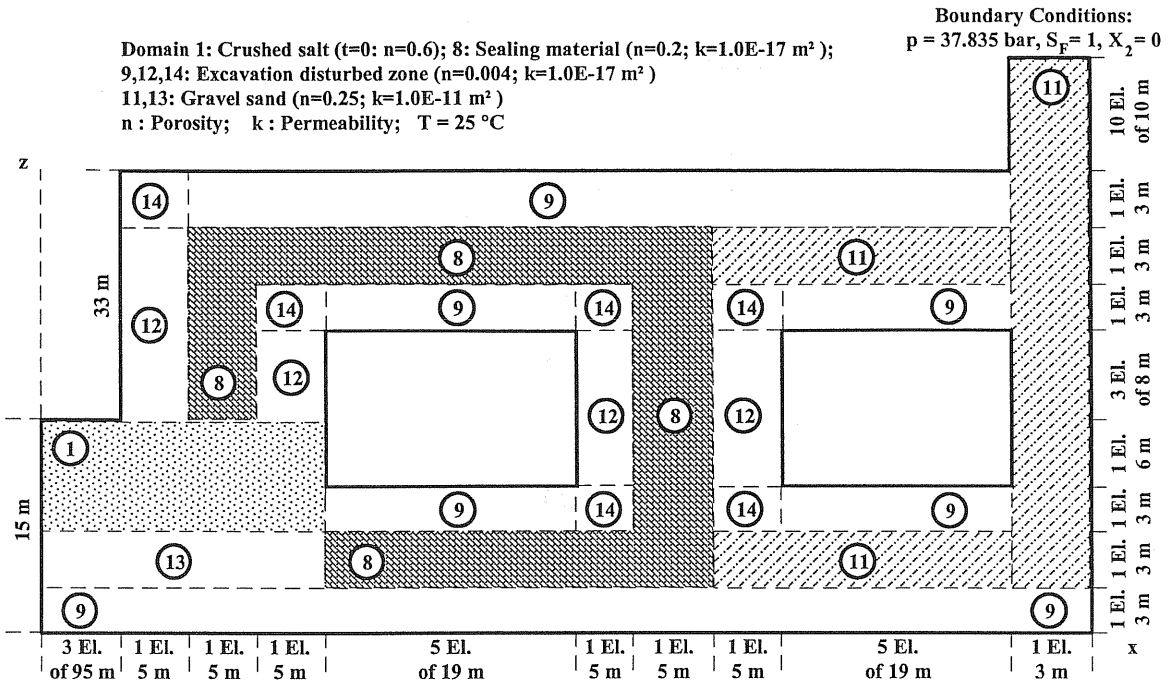β : dispersion length [m]; μ : dynamic viscosity [Pa·s]; ρ : density [kg/m^3]

Subscripts

G : gas phase; F : liquid phase
1 : primary liquid component (brine); 2 :secondary liquid component (tracer or nuclide)

References

/JAV 96B/ Javeri, V.: a contribution in GRS-129 (Dec. 1996)
/JAV 96C/ Javeri, V.: GRS-A-2389 (Oct. 1996)
/JAV 97B/ Javeri, V.: GRS-A-2441 (April 1997)
/PRU 91/   Pruess, K.: LBL-29400 (May 1991)
/PRU 91A/ Pruess, K.: LBL-31114 (Aug. 1991)
/PRU 93/   Pruess, K.: LBL-32505 (Sept. 1993)

Domain 1: Crushed salt (t=0: n=0.6); **8:** Sealing material (n=0.2; k=1.0E-17 m²);
9,12,14: Excavation disturbed zone (n=0.004; k=1.0E-17 m²)
11,13: Gravel sand (n=0.25; k=1.0E-11 m²)
n : Porosity; k : Permeability; T = 25 °C

Boundary Conditions:
p = 37.835 bar, S_F= 1, X_2 = 0

Domain 1: Chamber without gas source, variable porosity, Volume = 40500 m³, nuclide mass = 1.0E+04 kg
Domain 13: Chamber with gas source, constant porosity, Volume = 500 m³
Breadth in y-direction : 4 m ; Initial condition : p = 1 bar, S_F= 0.005

Figure 1 : Two dimensional network of a repository

Gas and Nuclide Transport in a 2-Dim. Repository
(Brine Inflow; C-Ref: FL1: 5E-5; FL2: 5E-4; FL3: 5E-3/Year)

Case : Chamber
FL1:Voidvol
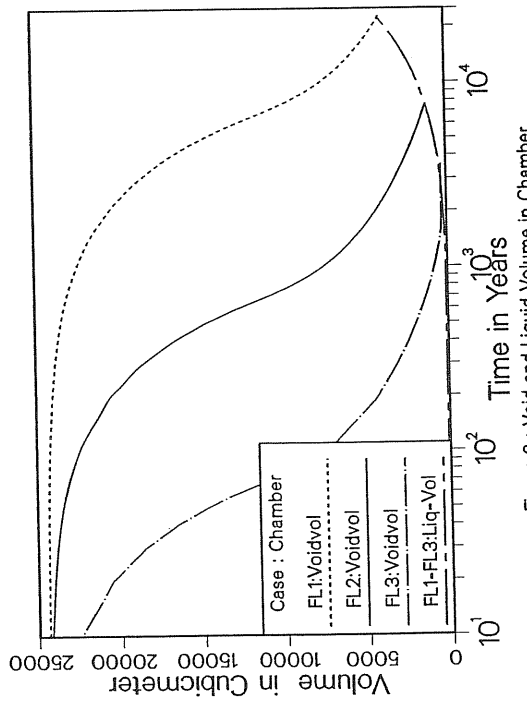FL2:Voidvol
FL3:Voidvol
FL1-FL3:Liq-Vol

Figure 2 : Void and Liquid Volume in Chamber

Gas und Nuclide Transport in a 2-Dim. Repository Network
(Brine Inflow;Chamber:Vol=41000 Cubicmeter,Init.Por=60 %)

Case: C-Ref
FL1:5E-5/Year
FL2:5E-4/Year
FL3:5E-3/Year
FL1:5E-5/Year
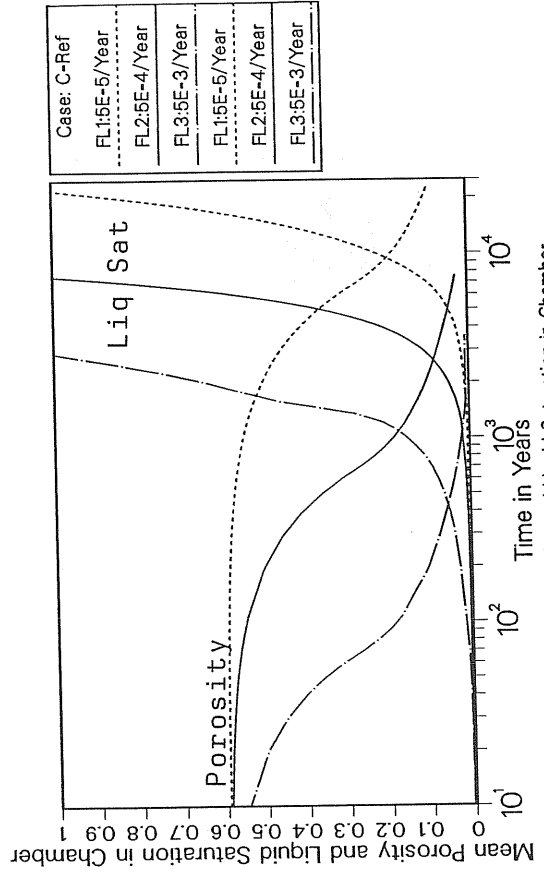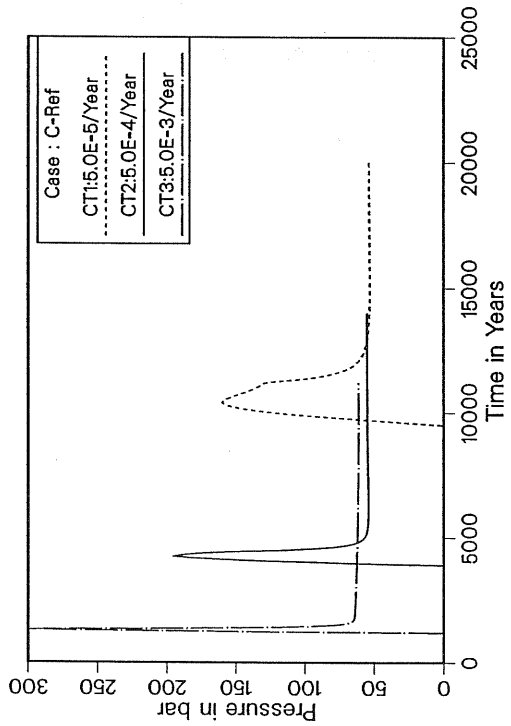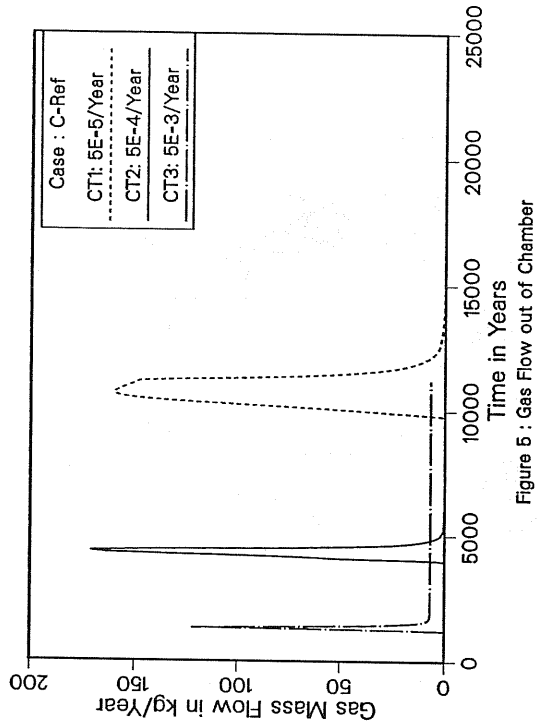FL2:5E-4/Year
FL3:5E-3/Year

Liq Sat

Porosity

Figure 3 : Mean Porosity and Liquid Saturation in Chamber

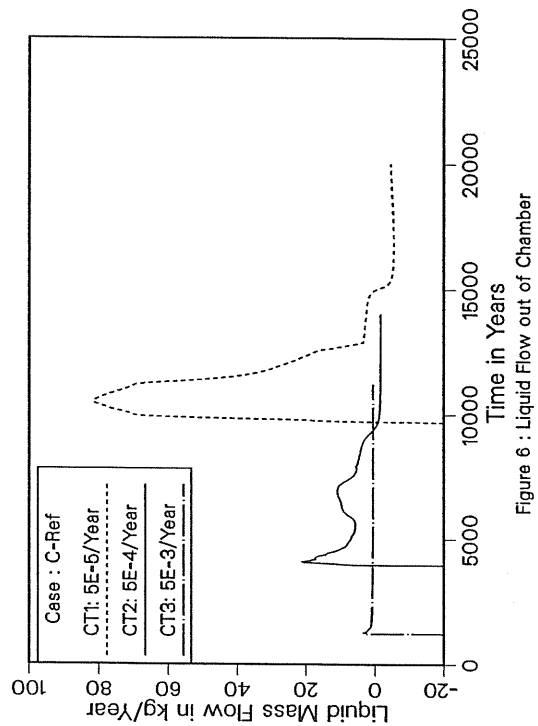Gas and Nuclide Transport in a 2-Dim. Repository Network
(Pressure in Chamber, x = 0 to 300 m, z = upper 9 m)

Case : C-Ref
CT1:5.0E-5/Year
CT2:5.0E-4/Year
CT3:5.0E-3/Year

Pressure in bar

300 250 200 150 100 50 0

Time in Years

Figure 4 : Chamber Pressure

Gas and Nuclide Transport in a 2-Dim. Repository Network
(Outflow {positive} from the Chamber)

Case : C-Ref
CT1: 5E-5/Year
CT2: 5E-4/Year
CT3: 5E-3/Year

Gas Mass Flow in Kg/Year

200 150 100 50 0

Time in Years

Figure 5 : Gas Flow out of Chamber

Gas and Nuclide Transport in a 2-Dim. Repository Network
(Outflow {positive} from the Chamber)

Case : C-Ref
CT1: 5E-5/Year
CT2: 5E-4/Year
CT3: 5E-3/Year

Liquid Mass Flow in Kg/Year

100 80 60 40 20 0 -20

Time in Years

Figure 6 : Liquid Flow out of Chamber

Gas and Nuclide Transport in a 2 -Dim. Repository Network
(Brine Outflow; Initial Nuclide Mass in Chamber:10000 kg)

Case : C-Ref
CT1: 5E-5/Year
CT2: 5E-4/Year
CT3: 5E-3/Year

Nuclide Removal from the Chamber in kg

1000 800 600 400 200 0

Time in Years

Figure 7 : Nuclide Removal from Chamber

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