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Development of an Analysis Program for Gas Migration in Geosphere

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1. Introduction

A proper understanding of gas migration processes is fundamental to both the qualitative discussion of gas migration in assessments of repository performance and the development of computational models to quantify effects on performance. In order to understand the consequences of gas release to the biosphere, it is also necessary to develop models of the transport of gas through a repository and the geosphere. A finite-element program to model two-phase flow of gas and groundwater in geosphere has been developed. This program can be used to evaluate the degree of overpressurization that will occur in the repository. It can also be used to estimate the time taken for gas to be released from the repository, the time taken for gas to migrate to the surface and the fluxes of gas to the biosphere. The influence of gas generation on the resaturation of the repository can also be examined.

2. Porous medium continuum flow model

2.1. Theoretical formulation

Gas migration through the geosphere of a radioactive waste repository can be modeled by multi-phase flow in porous media. The porous medium and the fluids are treated as continua in this approach, with no explicit representation of the phase boundaries between them. The presence of gas and groundwater is indicated by the volume fraction occupied by each.

For two-phase flow in a porous medium, such as the gas and groundwater flow around a waste repository, equations for the mass conservation for each phase are combined with a modified form of Darcy's equation, which includes the effects of relative permeabilities and capillary pressures:

$$-\left(\rho_w^{cw}\frac{dS_w}{dP_{cgw}}+\rho_g^{cw}\frac{dS_g}{dP_{cgw}}\right)n\frac{\partial P_w}{\partial t}+\left(\rho_w^{cw}\frac{dS_w}{dP_{cgw}}+\rho_g^{cw}\frac{dS_g}{dP_{cgw}}\right)n\frac{\partial P_g}{\partial t}$$
$$-\nabla\cdot\left[\rho_w^{cw}\frac{\mathbf{k}_w}{\mu_w}\cdot\nabla(P_w+\rho_w gz)\right]-\nabla\cdot\left[\rho_g^{cw}\frac{\mathbf{k}_g}{\mu_g}\cdot\nabla(P_g+\rho_g gz)\right]$$
$$=-nS_w\frac{\partial\rho_w^{cw}}{\partial t}-nS_g\frac{\partial\rho_g^{cw}}{\partial t}+\rho_w^{cw}q_w+\rho_g^{cw}q_g \tag{1}$$

$$-\left(\rho_w^{cg}\frac{dS_w}{dP_{cgw}}+\rho_g^{cg}\frac{dS_g}{dP_{cgw}}\right)n\frac{\partial P_w}{\partial t}+\left(\rho_w^{cg}\frac{dS_w}{dP_{cgw}}+\rho_g^{cg}\frac{dS_g}{dP_{cgw}}\right)n\frac{\partial P_g}{\partial t}$$
$$-\nabla\left[\rho_w^{cg}\frac{\mathbf{k}_w}{\mu_w}\cdot\nabla(P_w+\rho_w gz)\right]-\nabla\left[\rho_g^{cg}\frac{\mathbf{k}_g}{\mu_g}\nabla(P_g+\rho_g gz)\right]$$
$$=-nS_w\frac{\partial\rho_w^{cg}}{\partial t}-nS_g\frac{\partial\rho_g^{cg}}{\partial t}+\rho_w^{cg}q_w+\rho_g^{cg}q_g \tag{2}$$

Where superscript c is fluid component, subscript is fluid phase('w' for water, 'g' for gas), n is porosity, S is degree of fluid saturation, ρ is density, q is source or sink velocity. P_{cqw} is the capillary pressure, that is the difference between the gas and water pressures in the porous medium. k is effective permeability tensor (k=k_r k_{sat}). k_{sat} is saturated intrinsic permeability tensor of geosphere medium. Fluid saturations(S) and relative permeabilities (k_r) are functions of capillary pressure (P_{cqw}) and are represented by Van Genuchten model [1] in this program.

2.2. Numerical formulation

The governing equations (1) and (2) are discretized using the Galerkin finite-element method and Green's theorem [2], in which the solution variables are represented by discrete values on a grid constructed over the domain of interest. For equation (1), it is represented as follows:

$$-\int_R N_I\left(\rho_w^{cw}\frac{dS_w}{dP_{cgw}}+\rho_g^{cw}\frac{dS_g}{dP_{cgw}}\right)n\frac{\partial P_w}{\partial t}dR+\int_R N_I\left(\rho_w^{cw}\frac{dS_w}{dP_{cgw}}+\rho_g^{cw}\frac{dS_g}{dP_{cgw}}\right)n\frac{\partial P_g}{\partial t}dR$$
$$+\int_R\nabla N_I\cdot\left[\rho_w^{cw}\frac{\mathbf{k}_w}{\mu_w}\cdot\nabla(P_w+\rho_w gz)\right]dR+\int_R\nabla N_I\left[\rho_g^{cw}\frac{\mathbf{k}_g}{\mu_g}\cdot\nabla(P_g+\rho_g gz)\right]dR$$
$$=-\int_R N_I\left(nS_w\frac{\partial\rho_w^{cw}}{\partial t}+nS_g\frac{\partial\rho_g^{cw}}{\partial t}\right)dR+\int_R N_I(\rho_w^{cw}q_w+\rho_g^{cw}q_g)dR$$
$$+\int_B N_I\mathbf{n}\cdot\left[\rho_g^{cw}\frac{\mathbf{k}_g}{\mu_g}\nabla(P_g+\rho_g gz)\right]dB+\int_B N_I\mathbf{n}\left[\rho_g^{cw}\frac{\mathbf{k}_g}{\mu_g}\nabla(P_g+\rho_g gz)\right]dB \qquad I=1,2,3,\cdots,NN \tag{3}$$

The resulting non-linear systems of matrix equations are numerically solved by the use of static/dynamic incremental Picard method [3]. The linear solver used in this program is an iterative non-symmetric preconditioned conjugate gradient (NSPCG) algorithm [4].

3. Application

An illustrative gas migration calculation using the developed numerical model has been carried out in order to assess the extent of any build up of pressure and the timescales both for the build up of pressure and resaturation by groundwater of the repository. Fig. 1 shows vertical cross section and finite element mesh of the model domain. Hydrogeological properties of the model materials, groundwater, and gas used in the numerical simulation are summarized in Table 1. Gas generation rate is assumed as 2.37 x 10^{-11} kg/m^3/s in this simulation. Some of the results from this simulation are showed in Fig. 2~4. Spatial distribution and temporal change of gas pressure and gas saturation in the model domain are illustrated graphically in these Figures, respectively.

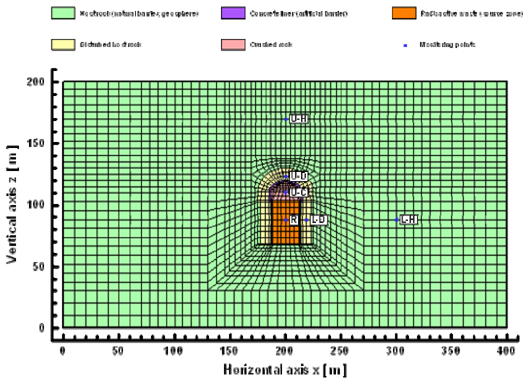


Figure 1. Vertical cross section and finite element mesh of the model domain

Table 1. Properties of the model materials, groundwater, and gas used in the numerical simulations.

Property	Host rock	Disturbed host rock	Concrete liner	Crushed rock	Radioactive waste zone
Porosity	3.50×10^{-3}	3.50×10^{-2}	1.50×10^{-1}	3.00×10^{-1}	6.90×10^{-1}
Saturated hydraulic conductivity [m/s]	$4.46 \times$ properties of the model materials, groundwater10^{-8}	4.46×10^{-6}	1.00×10^{-10}	1.00×10^{-4}	1.00×10^{-5}
Compressibility of water [Pa^{-1}]	4.40×10^{-10}				
Density of water [kg/m^3]	1.00×10^{3}				
	Dynamic viscosity of water [Pa s]				
Molar mass of water [kg/mole]	1.80×10^{-2}				
Dynamic viscosity of hydrogen gas [Pa s]	8.96×10^{-6}				
Molar mass of hydrogen gas [kg/mole]	2.00×10^{-3}				
Fluid pressure at STD [Pa] = 1 atm	1.00×10^{5}				
Temperature at STD [K]	298.15				
Gravitational acceleration constant [m/s^2]	9.81				

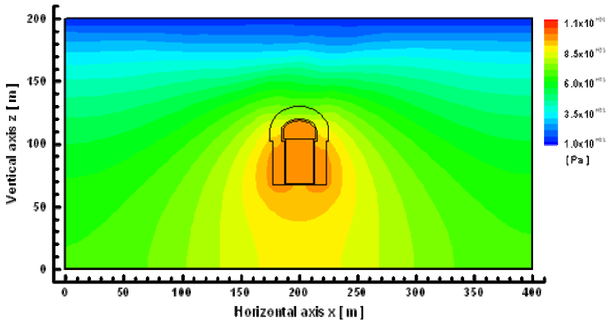


Figure 2. Spatial distribution of hydrogen gas pressure in the model domain after 127 days of gas generation

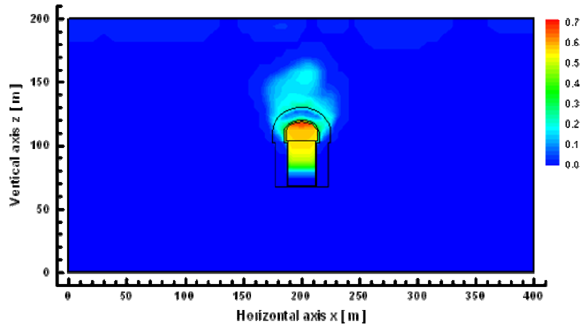
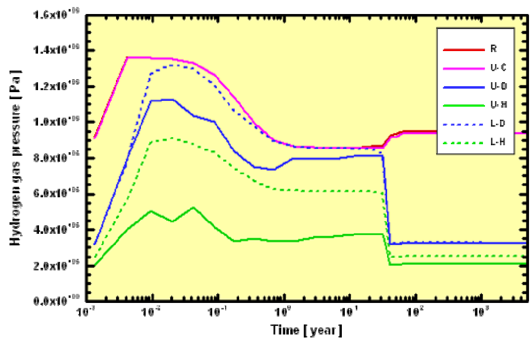


Figure 3. Spatial distribution of hydrogen gas saturation in the model domain after 127 days of gas generation



$1.00 \times$

Figure 4. Temporal change of hydrogen gas pressure at the six different monitoring points in the model domain during gas generation

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