Implementation of Non-isothermal Two-phase Flow Model Into COMSOL Multiphysics

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1. Introduction

In the case of a repository for radioactive waste, flow of ground water and gas is the key issue for the integrity of engineered barrier system (EBS). The intention of disposal is to provide sufficient isolation of radioactive wastes from reaching humans and the environment as long as possible. In order to fulfill such a strenuous criterion successfully, the evaluation of the combined effects of groundwater flow through the EBS and thermal loading from the decaying waste on the performance of the repository is important [1].

Recently, KAERI proposed the concept of the process-based total system performance assessment model for a geological disposal system which is called APro (Advanced Process-based total system performance assessment framework for a geological disposal system) [2]. Because COMSOL Multiphysics is one of the main code for APro, thermal-hydraulic model using COMSOL Multiphysics should be required.

Therefore, in this study, we implemented non-isothermal two-phase flow model into COMSOL Multiphysics and verified the numerical model compared with the results of TOUGH2.

2. Governing equation

2.1 Basic assumptions

Basic assumptions for the governing equation of non-isothermal two-phase fluid flow are defined as follows:

- Local thermodynamic (mechanical, thermal, and chemical) equilibrium
- Rigid solid phase
- Two-phase flow consisting of a liquid phase and a gas phase
- Two components being present in each phase: water and air
- Compositional model which allows a transfer of components from one phase into the other
- Negligible influence of dispersion and diffusion

2.2 Mass balance equation

Mass balance equation for arbitrary subdomain V_n of the flow system which is bounded by the closed surface Γ_n is as follows:

$$\frac{d}{dt}\int_{Vn} M^{\kappa} dV_n = \int_{\Gamma n} \mathbf{F}^{\kappa} \bullet \mathbf{n} d\Gamma_n + \int_{Vn} q^{\kappa} dV_n \quad (1)$$

where κ is the mass component (water and air).

Mass accumulation term M^{κ} is as follows:

$$M^{\kappa} = \phi \sum_{\beta} S_{\beta} \rho_{\beta} X_{\beta}^{\kappa} \quad (2)$$

where β is fluid phase (liquid and gas), Φ is porosity, S_β is saturation of phase β, ρ_β is density of phase β, and X_{β}^{κ} is mass fraction of component κ present in phase β.

Only advection is considered for mass flux term F^{κ} based on multi-phase Darcy's law.

$$\mathbf{F}^{\kappa}\Big|_{adv} = \sum_{\beta} X_{\beta}^{\kappa} \mathbf{F}_{\beta} \quad (3)$$

$$\mathbf{F}_{\beta} = \rho_{\beta} \mathbf{u}_{\beta} = -k \frac{k_{r\beta} \rho_{\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} \mathbf{g}) \quad (4)$$

where u_β is Darcy velocity (volumetric flux) in phase β, k is absolute permeability (intrinsic permeability), $k_{r\beta}$ is relative permeability to phase β, and μ_β is viscosity in phase β.

2.3 Energy balance equation

The form of energy balance equation is similar with the Eq. (1).

Heat accumulation term M^H is as follows:

$$M^H = (1-\phi)\rho_R C_R T + \phi \sum_\beta S_\beta \rho_\beta u_\beta \qquad (5)$$

where Φ is porosity, ρ_R is grain density of rock mass, C_R is specific heat of rock mass, and u_β is specific internal energy in phase β.

Heat flux term F^H is as follows:

$$\mathbf{F}^H = -\lambda \nabla T + \sum_\beta h_\beta \mathbf{F}_\beta \qquad (6)$$

where λ is thermal conductivity, and h_β is specific enthalpy in phase β.

3. Verification

We verified COMSOL Multiphysics compared with TOUGH2 results using 1D unsaturated domain. Fig. 1 shows the geometry, initial condition, and boundary conditions of 1D unsaturated flow model.

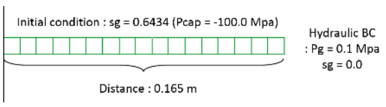

Fig. 1. Schematic view of 1D unsaturated domain.

Table 1 shows properties of the unsaturated domain.

Table 1. Properties of the unsaturated domain

Properties			Value
Porosity			0.438
Permeability (m^2)			6.4E-21
Pore compressibility (Pa^{-1})			1.0E-10
Relative permeability (Corey's curve)	$k_{rl} = \hat{S}^4$	S_{lr}	0.0
		S_{gr}	0.0
	$k_{rg} = (1-\hat{S})^2(1-\hat{S}^2)$	λ	4.0
Capillary pressure (Van Genuchten curve)	$P_c = -P_0([S^*]^{-1/\lambda}-1)^{1-\lambda}$	λ	0.3
		S_{lr}	0.0
		P_0	1.08e-7
		P_{max}	1.0E+15

Fig. 2 shows the distribution of liquid saturation in 1D unsaturated flow model. Dot means TOUGH2 results and line means COMSOL Multiphysics results. As shown in Fig. 2, the results of COMSOL Multiphysics are well matched with the results of TOUGH2.

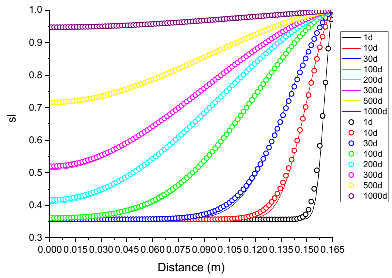

Fig. 2. Distribution of liquid saturation in 1D unsaturated flow model.

4. Conclusion

In this study, we implemented non-isothermal two-phase flow model into COMSOL Multiphysics and verified the numerical model compared with the results of TOUGH2 using 1D unsaturated domain. For further work, more comprehensive verifications and validations will be conducted. After verifications and validations, we will embed this model in the process-based total system performance assessment model for a geological disposal system (APro).

ACKNOWLEDGEMENT

This work was supported by the Nuclear Research and Development Program (No. 2017M2A8A5014856) of the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (MSIT).

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