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Research Paper

Optimal initial condition of a bentonite buffer with regard to thermal behavior in a high-level radioactive waste repository

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ABSTRACT

In this study, a numerical model was established using the coupled relationship between the initial conditions of dry density and thermal–hydraulic properties of the compacted bentonite buffer in high-level waste repositories. In addition, we applied the firefly algorithm to identify the optimal initial condition of the buffer, based on the numerical model. Results showed the minimum peak temperature was 77.89 °C at the optimal initial condition where the dry density was 1683 kg/m^3. The results were verified using the convergence test and parametric study. This finding gives a guideline for producing a bentonite buffer condition in the design of a repository.

1. Introduction

A deep geological repository is among the reliable systems of high-level radioactive waste (HLW) disposal, safely maintaining HLW at depths of more than 500 m underground and permanently isolating it from human life. A repository is composed of canister, buffer, backfill, and near-field rock, hence serving as an engineered barrier system. The buffer, which is an important component of a repository, protects the container from the inflow of groundwater and restrains the release of radionuclides. The buffer is placed between the waste canisters and surrounding rock and will be saturated by the nearby groundwater while it is subjected to high temperatures caused by the decay heat of the radioactive waste. Thus, a buffer requires high thermal conductivity to effectively release decay heat from the canister and low hydraulic conductivity to minimize groundwater inflow from the saturated rock. Countries adopting a deep geological repository have selected a candidate or reference bentonite to be used as the buffer material either alone or mixed with different additives [1]. As bentonite is a clay mineral that is fundamentally composed of smectites containing large amounts of montmorillonite, it becomes plastic when mixed with water and has extraordinary expansive properties. The smectites are composed of structural units comprising two polyhedral tetrahedral coordination (T) layers, and a central octahedral layer, known as 2:1 silicates [2]. Depending on the exchangeable cations in the layers, two main classes of bentonite exist: a Na-type and a Ca-type. Sweden, Finland, Switzerland, and Japan consider Na-type bentonite as a buffer material candidate, while Ca-type bentonite is proposed as a reference buffer in Spain and Korea.

As the chemical and mineralogical structure of the bentonite is affected by its temperature variation, the thermal behavior of the buffer caused by the decay heat is important in the design process of the repository. Accordingly, a typical thermal criterion for a geological repository is that the maximum temperature of the buffer should remain below 100 °C during operation [3]. Thus, the deposition hole spacing and distance from the disposal tunnel should be determined using a thermal behavior analysis of the repository so as not to exceed this criterion. The thermal behavior is affected by not only the thermal but also the hydraulic properties of the buffer, as the inflow of groundwater in the buffer can affect the thermal behavior by varying its water content.

To satisfy the requirements of the buffer and the design criteria of the repository previously described, bentonite is used in the form of a highly compacted block. In general, the bentonite powders are compressed using the floating die method and a cold isostatic pressing technique is applied to form a compacted bentonite block. Considering that the repository is thoroughly isolated and access is restricted during the operation, the design factors of the buffer cannot be modified following installation. A buffer exhibits different behaviors even under the same ambient conditions depending on the initial design conditions, and thus the optimized buffer design conditions should be investigated

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to provide the highest long-term stability of the repository.

Accordingly, many researchers have studied the physical properties of a bentonite buffer. Properties and behavioral characteristics of compacted bentonite blocks have been experimentally investigated particularly with a focus on thermal [4–7] and hydraulic factors [8–11] for various types of reference buffers such as MX-80, FEBEX, and Kyungju. Furthermore, the coupled relationships of the physical properties of the compacted bentonite block have been implemented in previous studies on numerical simulations of the repository [12–16].

Although it is important to determine the optimal initial conditions of the buffer to maintain the thermal criterion of the repository as well as to minimize depositional hole spacing, there has been a lack of effort to identify the optimal initial conditions for the advantageous thermal behavior of the buffer. Thus, this study investigates the optimal initial conditions for the minimum peak temperature of the buffer by applying an optimization technique using a numerical model including the thermal and hydraulic property relationships of compacted bentonite.

2. Numerical analysis

2.1. Governing equation

Considering a situation of an HLW repository, a heat and fluid coupled analysis of porous media is needed for thermal behavior analysis. Thus, a commercial program, COMSOL Multiphysics 5.3a [17], in which a combined analysis of heat and fluid fully coupled flow is possible based on the finite element method, was used in this study. The Heat Transfer Module and Subsurface Flow Module of COMSOL Multiphysics were implemented and the governing equations of each module are as discussed in the following sections.

2.1.1. Heat transfer module

Heat transfer in a porous medium mainly occurs via heat conduction [18]. Accordingly, the governing equation considered in Heat Transfer Module is as follows:

$$-\lambda_i\cdot\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)+\rho_i\cdot c_i\cdot\frac{\partial T}{\partial t}+q_i=0\ (i=x,y,z) \tag{1}$$

where T is the temperature of the porous medium as a dependent variable, λ is the thermal conductivity of the medium, ρ is the density, c is the specific heat capacity, and q_i denotes the internal heat generation.

2.1.2. Subsurface flow module

For fluid flow in a bentonite buffer, the Richards equation [19] in the Subsurface Flow Module can be applied to both unsaturated and saturated flows in a porous medium. Eq. (2) defines the storage and retention models in variably saturated porous media and it can estimate the saturation according to the time, fluid pressure, and space [17,20].

$$\rho_f\cdot\left(\frac{C_m}{\rho_f\cdot g}+S_e\cdot S\right)\cdot\frac{\partial p}{\partial t}+\nabla\cdot\left[-\frac{\rho_f\cdot\kappa_s}{\mu}\cdot k_r\cdot(\nabla p+\rho_f\cdot g\cdot\nabla D)\right]=Q_m \tag{2}$$

where p is the pressure as a dependent variable, ρ_f is the fluid density, C_m denotes the specific moisture capacity, and g is the acceleration due to gravity. In addition, S represents the storage coefficient, S_e is the effective saturation, μ the fluid dynamic viscosity, k_r the relative permeability, k_s the intrinsic permeability, t the time, D the elevation, and Q_m specifies the fluid source (positive) or sink (negative). The specific storage is set as follows:

$$S=\rho_f\cdot g\cdot(\chi_p+\theta\chi_f) \tag{3}$$

where χ_p and χ_f are the compressibility of the solid particles and fluid, respectively, and θ is the volumetric water content defined as the volume of liquid per porous medium volume.

The relative permeability k_r is derived from the Van Genuchten closed-form model as follows [21]:

$$k_r=\begin{cases}S_e^L\left[1-\left(1-S_e^{\frac{1}{m}}\right)^m\right]^2 & for\ H_p<0\\ 1 & for\ H_p\geqslant 0\end{cases} \tag{4}$$

where m is a shape parameter for the retention curve of van Genuchten, expressed as 1 − (1/n), and S_e is defined as follows:

$$S_e=\begin{cases}\frac{S-S_r}{S_s-S_r}=\left[\frac{1}{1+|\alpha H_p|^n}\right]^m & for\ H_p<0\\ 1 & for\ H_p\geqslant 0\end{cases} \tag{5}$$

where S, S_r, and S_s are the current, maximum, and residual liquid degrees of saturation, respectively. The specific moisture capacity, C_m, is defined as follows:

$$C=\begin{cases}\frac{\alpha m}{1-m}(\theta_s-\theta_r)S_e^{\frac{1}{m}}\left(1-S_e^{\frac{1}{m}}\right)^m & for\ H_p<0\\ 0 & for\ H_p\geqslant 0\end{cases} \tag{6}$$

where θ_s and θ_r are the saturated and residual porosity, respectively. The parameters α, n, and L are calculated by fitting the van Genuchten equations using an experimentally measured water retention curve of the bentonite.

2.2. Verification

To verify the suitability of the numerical model, a numerical analysis using COMSOL Multiphysics 5.3a was performed and the results were compared to those of an analytical solution. Hodgkinson [22] suggested the analytical model which can be applicable to the decaying heat source generated from the canister in a HLW repository [23]. The decay heat decreases exponentially according to the half-life of the radioactive waste in the model where the temperature variation at a point away from the source and after the elapsed time caused by the heat sources can be expressed as Eq. (7):

$$T(R,z,t)=\frac{q_0\cdot e^{-kt}}{4\rho c\alpha}\int_0^t d\mu\cdot\frac{e^{-kt}}{\mu}\cdot\left\{erf\left(\frac{z+b}{2\sqrt{\alpha\mu}}\right)-erf\left(\frac{z+b}{2\sqrt{\alpha\mu}}\right)\right\}\int_0^r R'\cdot I_0\left(\frac{RR'}{2\alpha\mu}\right)\cdot\exp\left\{\frac{-(R^2+R'^2)}{4\alpha\mu}\right\}\cdot dR' \tag{7}$$

where b is the cylinder half length, r is the cylinder radius, and I_0 is a modified Bessel function. Also, R and z are the radial and axial coordinates, respectively. In addition, k is the decay constant, α is the thermal diffusivity, q_0 is the initial rate of heating per unit volume, and t is the time.

In comparing the numerical model results to the analytical solution, a two-dimensional (2D) axisymmetric finite element model was constructed by employing the geometry of the Korean Reference Disposal System [24] and the values of properties presented in Table 1. As in the case of the analytical solution, the boundary conditions and material properties of the numerical model were also fixed as constant values during the analysis.

Fig. 1 shows a comparison of the temperature variations of the

Table 1
Values of input data for verification.

	Property	Value	Reference
Input data	Thermal conductivity (λ)	2.427 W/(m·K)	Gibb et al. 2008 [23]
	Specific heat capacity (C_p)	2700 J/(kg·K)	
	Density (ρ)	820 kg/m^3	
	Radius of heat source (r)	0.51 m	Lee et al. 2014 [15]
	Height of heat source (B)	2.145 m	
Heat source	$S = Q_0\exp(-\lambda_e t)$ (Q_0 = 670 W/m^3, $T_{1/2}$ = 30 y)		Zhang et al. 2013 [44]