Integration of Thermal-Hydraulic Two-phase Flow Analysis to Evaluate Corrosion Behavior of Copper Canisters in Deep Geological Repository: HADESNU 1.1

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1. Introduction

Spent Nuclear Fuels (SNFs), which are accumulating on nuclear power plant sites in the Republic of Korea, need to be disposed of safely in a final disposal repository. For the performance assessment of the future Deep Geological Repository (DGR) system, Seoul National University has already developed a Finite Element Method (FEM)-based numerical model with Multiphysics Object Oriented Simulation Environment (MOOSE) framework – HADESNU (High-level radioActive waste Disposal Evaluation Simulator for Near-field evolUtion) – calculating Thermal-Hydraulic-Chemical-Electrochemical (THC-EC) coupled behaviors occurring in DGR environment [1-2].

The previous version of HADESNU (1.0) couples Thermal and Hydraulic (TH) physics with Chemical-Electrochemical (C-EC) corrosion module based on the simplified Richards' flow, which assumes the gas pressure has a constant value. However, this approach has limitation in describing more extreme conditions over 100 ℃, under which the gas phase becomes important regarding groundwater behaviors and subsequent corrosion mechanisms. Therefore, the two-phase flow approach should also be incorporated into the THC-EC coupled model to enable a more rigorous evaluation of its effects on corrosion behavior, thereby enabling the model to further describe the high-temperature conditions of DGR system that may arise from variations in SNFs disposal hole spacing or disposal density.

This study updates the previous HADESNU model into HADESNU 1.1, integrating the two-phase flow approach of TH modules with a C-EC corrosion module. To assess whether the model has been properly developed, the major calculation results are compared with the previous Richards' flow-based model under 100 ℃.

2. Methodologies

2.1. Governing Equation of Thermal Behavior

The thermal behavior of DGR environment can be described with the following energy conservation equation [2]:

$$\frac{\partial}{\partial t}\left[\left(\rho C_p\right)_{eff} T\right] - \nabla \cdot \left(\lambda_{eff} \nabla T\right) + J_{conv}^{liq} + J_{conv}^{gas} = Q \quad (1)$$

where the first term represents effective volumetric heat capacity with ρ of density, C_p of specific heat. The second term represents the heat conduction with λ_{eff} of effective thermal conductivity, while J_{conv}^{liq} represents the heat convection term of liquid phase. The two-phase flow adds the last term of J_{conv}^{gas} which describes the heat convection term of gas phase. The detail can be explained as follows [2]:

$$J_{conv}^{gas} = -\rho^g C_p^g \frac{\mathbf{k} k_{rel}^g}{\mu^g} \left(\nabla P^g - \rho^g g\right) \cdot \nabla T \quad (2)$$

where $\mathbf{k}$ represents the intrinsic permeability and k_{rel}^g the relative permeability of gas phase. This term enables the two-phase flow model to consider additional heat convection driven by gas pressure, describing the unsaturated high temperature condition under DGR environment.

2.2. Governing Equations of Hydraulic Behavior

The hydraulic behavior of DGR environment are governed by two mass balance equations. The first equation corresponds to the mass balance of groundwater; which is also included in Richards' flow approach [2]:

$$\frac{\partial}{\partial t}\left[\phi (S\rho)_{eff}\right] + \nabla \cdot \left(J_w^{A,l} + J_w^{A,g} + J_w^{D,g}\right) = Q \quad (3)$$

where the first term represents the water mass accumulation with ϕ of porosity and S of degree of saturation, while $J_w^{A,l}$ and $J_w^{D,g}$ represents the advective flux of liquid water and diffusive flux of water vapor. $J_w^{A,g}$ is the newly added term in two-phase flow approach describing advective flux of water vapor:

$$J_w^{A,g} = -\rho_w^g \frac{\mathbf{k}k_{rel}^g}{\mu^g}(\nabla P^g - \rho^g g) \quad (4)$$

the shape of which is similar with J_{conv}^{gas} above.

The second mass balance equation is added for the air – which was not included in Richards' flow [2]:

$$\frac{\partial}{\partial t}\left[\phi(S\rho)_{gas}\right] + \nabla \cdot \left(J_a^{A,g} + J_a^{D,g}\right) = Q \quad (5)$$

where $J_a^{A,g}$ and $J_a^{D,g}$ represent advective and diffusive flux of air. Two terms can be described with more details [2]:

$$J_a^{A,g} = -\rho_a^g \frac{\mathbf{k}k_{rel}^g}{\mu^g}(\nabla P^g - \rho^g g) \quad (6)$$

$$J_a^{D,g} \approx -J_w^{D,g} \approx -\left(D_{pv}\nabla P^{cap} + f_{Tv}D_{Tv}\nabla T\right) \quad (7)$$

where D_{pv} is the isothermal vapor diffusivity, f_{Tv} is the thermal diffusion enhancement factor and D_{Tv} is thermal vapor diffusivity.

These advective and diffusive terms describe the mass flow and redistribution of gas phases, reflecting the evaporation, condensation and migration of air and vapor more rigorously than Richards' flow approach.

2.3. Governing Equations of Chemical and Electrochemical Behaviors

The C-EC behaviors under DGR environment can be described as the transport of chemical species, while involving the electrochemical redox reactions. The transport of the species can be described [1]:

$$\phi\frac{\partial}{\partial t}(SC_i) - \nabla \cdot [\phi\tau SD\nabla C_i] - \nabla \cdot J = 0 \quad (8)$$

where τ represents the tortuosity and D represents the diffusion coefficient. J in the third term describes the advection with more details as follows [1]:

$$J = \frac{\mathbf{k}k_{rel}}{\mu}(\nabla P^{cap} - \rho g)C_i \quad (9)$$

for the concentration of each species i. The redox reactions describing the corrosion of copper canister can be summarized as shown in Table I.

Table 1. Reactions used in HADESNU 1.1 [1].

No.	Reaction
1	$Cu+2Cl^- \leftrightarrow CuCl_2^- + e^-$
2	$2Cu + HS^- \leftrightarrow Cu_2S + H^+ + 2e^-$
3	$O_2 + 2H_2O + 4e^- \leftrightarrow 4OH^-$
4	$HS^- + H_2O + e^- \leftrightarrow 1/2H_2 + HS^- + OH^-$
5	$Cu^{2+} + 2Cl^- + e^- \leftrightarrow CuCl_2^-$
6	$H_2O + e^- \leftrightarrow 1/2H_2 + OH^-$

2.4. Geometry and Calculation Condition

The calculation of HADESNU aims to describe the DGR system of Improved KAERI Reference Disposal System (KRS+), especially for 1/4 of one disposal hole in three dimensions. The specification of geometry is described in Fig 1.

The same conditions of normal disposal environment – described in the previous literature dealing with Richards' flow [3] – are applied into both Richards' flow and two-phase flow approach.

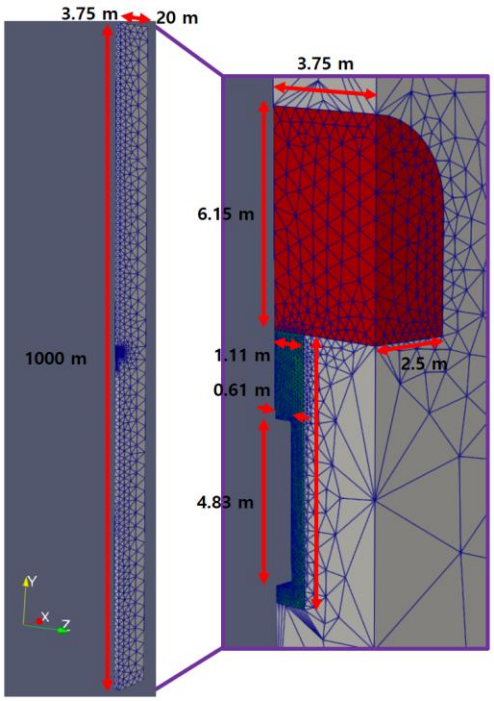


Fig 1. Geometry of 3D 1/4 disposal hole used for HADESNU 1.1 Calculation.

3. Results and Discussion

Fig 2 and 3 show the profile of temperature and degree of saturation over time at the top center and corner of the canister. The similar results were derived from both Richards' flow and two-phase flow approach, with the peak temperature of around 97 °C and the lowest degree of saturation to be around 0.2 ~ 0.3.

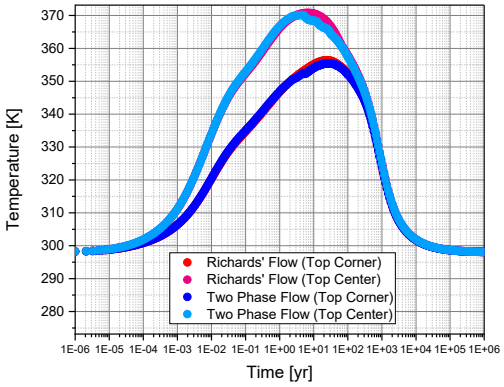


Fig 2. Calculation result of HADESNU 1.1: Temperature over time at top center/corner of the canister.

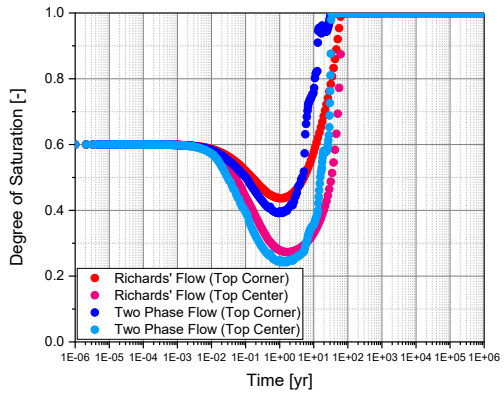


Fig 3. Calculation result of HADESNU 1.1: Degree of saturation over time at top center/corner of the canister.

The corrosion potential calculated by HADESNU 1.1 at each point is shown in Fig 4. Two approaches derives almost same values and trends of the corrosion potential over time, confirming that the two-phase flow approach describes reasonable behavior of the normal condition under 100 ℃.

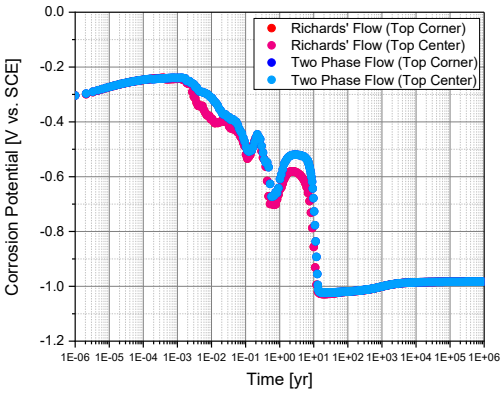


Fig 4. Calculation result of HADESNU 1.1: Corrosion potential over time at top center/corner of the canister.

4. Conclusion

This study aimed to integrate the Two Phase Flow approach of DGR system's TH behaviors with C-EC behaviors for copper canister's corrosion. Under the normal condition below 100 ℃, two approach showed almost similar calculation results. With the reasonable calculation of two-phase flow approach, this study has its meaning of establishing the foundation to analyze the impact of high-temperature condition on copper canisters' corrosion behavior under DGR system.

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