New High Fidelity Multi-physics FEM based Code to Simulate the Boron Hide-out within CRUD Layer

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1. Introduction

During the long term high power operation of nuclear power plant, axial offset of power distribution has occurred. CRUD, Chalk River Unidentified Deposit or Corrosion Related Unidentified Deposit, was observed in that situation on the surface of fuel rods, and boron hideout has been suggested as one of the reason for the axial shift [1,2].

The lithium history in reactor coolant system during reactor operation is one of the proof for boron hideout [2]. However, for the validation of these phenomena, more basic analysis should be conducted, as experimentally and computationally. Experimental validation for the CRUD and boron hideout is extremely hard to conduct because the boron hideout will occur at only high temperature and pressure condition with requirement of real-time measurement. Computational validation can easily solve these amount of boron hideout, so modeling approach is necessary.

New 2D macro-scale model for solving multi-physics within the CRUD layer, to predict the amount of boron hideout was developed. Finite element method (FEM) was used by using PETSc and LibMesh libraries. Heat transfer, capillary flow, solute transport and chemistry within the CRUD layer were calculated. Full core simulation system with parallel calculation was constructed with C++ language.

2. Model

2.1.Geometry and target NPP operation

Uniform CRUD layer with 50um thickness was assumed as target operation. The height of CRUD layer is 3.65 m. The CRUD layer is porous with uniform porosity, and the CRUD layer and steam chimney in the CRUD layer was averaged as one domain by using volume-averaged method. The geometrical information for the CRUD such as chimney density and porosity, was used from previous researches [4,6,7]. The NPP operation conditions were also used from these researches, such as cladding heat flux of 1MW/m^2, coolant temperature 600K, coolant pressure 153.42bar, near the EOC species concentration as unit of mol/m^3.

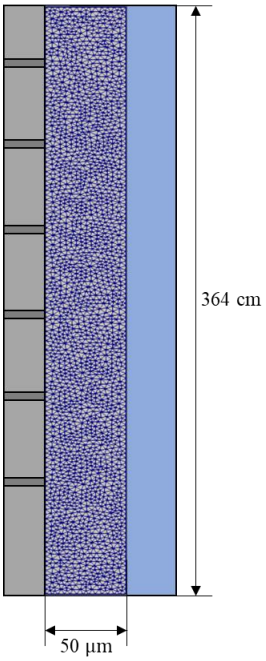

Figure 1. The geometry of uniform CRUD layer on the surface of cladding.

Table 1. The boundary conditions and initial conditions used in this model

Condition	*Value*	*Unit*
$Q_{cladding}$	*1*	*MW/m^2*
$T_{bulk\ coolant}$	*600*	*K*
$P_{bulk\ coolant}$	*153.42*	*bar*
$B(OH)_3$	*19.17*	*mol/m^3*
OH^-	*2.94E-2*	*mol/m^3*

$B(OH)_4^-$	*0.211E-2*	*mol/m³*
Li^+	*5.14E-2*	*mol/m³*
H^+	*4.17E-5*	*mol/m³*
$LiBO_2$	*1E-30*	*mol/m³*

2.2.Multi-physics in CRUD layer

In heat transfer phenomenon, the coolant within the CRUD layer will evaporate according to temperature difference with saturation temperature. This will be used for calculating sub-cooled nucleate boiling heat sink. The heat will from the cladding, and it will move toward coolant interface, and during the travel, it will lose some portion of itself by evaporation. From the amount of SNB heat sink, mass conservation with SNB mass sink was calculated as steady state, and this will leads pressure drop across CRUD layer. These pressure drop will leads the Darcy flow through CRUD layer, and it will leads influence on heat transfer and solute transport. Steady state mass transport of solute via diffusion and convection within the CRUD layer with three chemical reactions of boron and water was calculated to determine the amount of boron hideout for give situation.

2.3.Heat transfer model

From the energy conservation equation with steady state, the heat transfer model within the CRUD layer with heat sink was derived. The conduction of heat through CRUD layer and convection of heat through Darcy flow within the CRUD layer were derived. The heat sink term was re-derived from the heat sink term of MAMBA-3D, by matching missed unit in MAMBA-3D, especially removing permeability term [6]. The boundary condition was used the heat flux condition at cladding interface and convective heat sink at coolant interface. The properties for heat transfer model was volume-averaged between CRUD and water, and some correlation was adjusted for reliable range. The thermal conductivity of these effective domain was from the correlation of Short et al.'s model[7] and the evaporative heat transfer coefficient was from the correlation of Henshaw et al.'s model[4].

$$\nabla\left(\frac{k_{th}^{eff}}{c_v^{eff}}\nabla T\right)+\tau\left(\frac{\kappa}{\mu\varepsilon}\nabla P\right)\nabla T-\varepsilon\frac{2\pi r_c n_c h_e(T-T_{sat})}{c_v}=0 \quad (1)$$

2.4.Capillary flow model

From the mass conservation equation with mass sink at steady state, the pressure equation was derived for initial state of governing equation. From the steady-state evaporative heat sink in heat transfer model, the evaporative mass sink term of coolant was derived by using vaporization enthalpy and Darcy flow eqeuation. Boundary condition at cladding interface means no flux condition, and that at coolant interface is ideal provision of mass by using Dirichlet boundary condition. The properties such as viscosity, permeability was form the correlation of Short et al.'s model[7], NIST water properties data and the model of meso-scale[5]..

$$\nabla^2 P \;-\; 2\varepsilon\pi r_c n_c h_e(T-T_{sat})\frac{\mu}{h_{fg}\rho\kappa}=0 \quad (2)$$

2.5.Solute transport and chemistry model

From the Fick's second law with diffusion and convection term at steady state, the chemical reaction term was added for three chemical reaction of boron species and water ions. Boundary condition at cladding interface was used as no flux condition, and that at coolant interface was Dirichlet boundary condition with that in capillary flow model. The material properties and chemical reaction data were from the model of meso-scale[5].

$$\nabla(D_i\nabla C)\;-\;\nabla(VC_i)\;-\;\sum RR_j=0 \quad (3)$$

2.6. Construction of code and parallel calculation interface for quarter core

By using C++ language, PETSc numerical library and LibMesh FEM library, the FEM based numerical code was constructed. The parallel calculation interface was constructed to conduct the quarter core calculation by using MPI interface. Each processor will calculate the internal physics of CRUD layer for each assigned fuel rod, sub-channel and assembly. Although there is no sufficient input data to apply different input value for each fuel rod and sub-channel, the interface has been updated for future application.

3. Result and discussion

Figure 1 shows the distribution of temperature, SNB heat flux and pressure distribution within the CRUD layer. The temperature distribution was in range from 613K to 632K and it is well matched with previous researches. The pressure drop across the CRUD layer was about 3kPa to 4kPa, while previous researches showed the 1kPa to 2kPa. The order of SNB heat flux was similar with other CRUD code. Figure 2 and Figure 3 show the amount of concentration of each species within the CRUD layer by using EOC coolant

concentration conditions. The goal of the solute transport and chemistry model is generating amount of boron hideout by using full consideration of LiBO2 precipitation reaction, and the result of LiBO2 shows the precipitated value of 0.03mg/cm3 while that is MAMBA-3D code shows near 0.1~0.2 mg/cm3 in averaged and BOA is 0.1 mg/cm3. By using effect of evaporation in solute transport and chemistry, new source term can be considered in this model. The evaporation will leads the local enrichment of species at the evaporation point, and it will leads some increase of amount and pattern of LiBO2 precipitation. The result in this case shows the precipitation amount of 0.15mg/cm3.

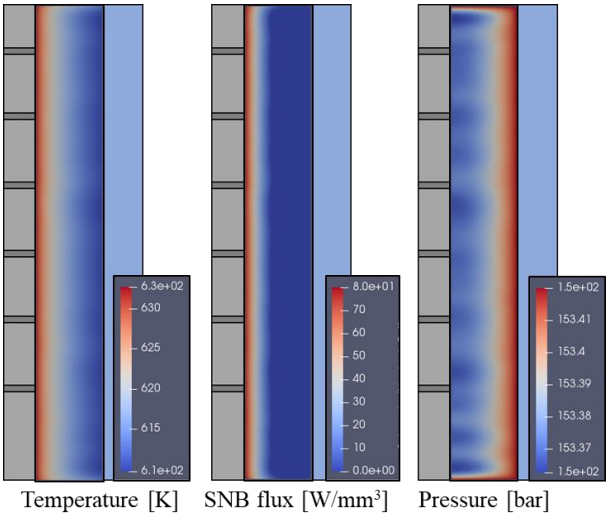

Figure 2. Results of temperature, SNB flux, and pressure distribution within the CRUD layer.

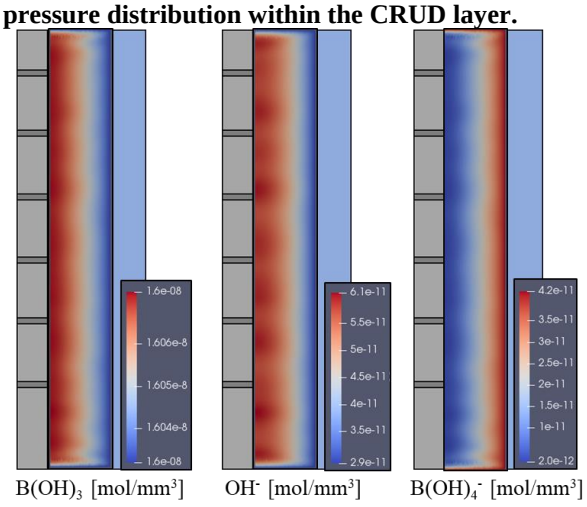

Figure 3. Result of B(OH)3, OH-, B(OH)4- concentration within the CRUD layer.

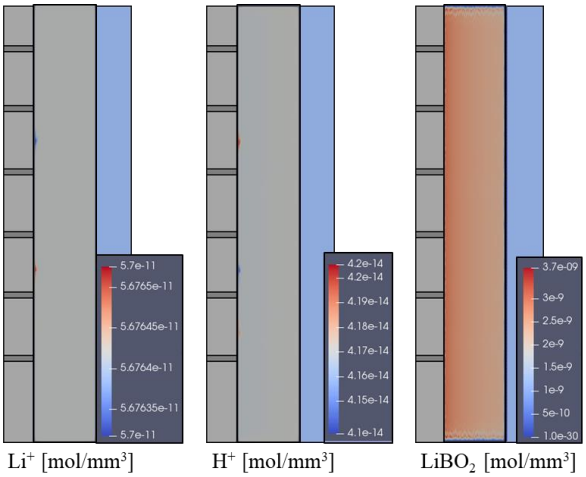

Figure 4. Result of Li+, H+, LiBO2 concentration within the CRUD layer.

4. Conclusion

New FEM based 2D macro-scale multi-physics code was developed by using PETSc and LibMesh libraries to predict the boron hideout within the CRUD layer. The results of temperature, SNB flux, pressure and boron mass show similar order of result with other code, but different distribution with MAMBA-3D.

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