A COUPLED TH/NEUTRONICS/CRUD FRAMEWORK IN PREDICTION OF CIPS PHENOMENON

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ABSTRACT

A coupled TH/Neutronics/CRUD framework, which is able to simulate the CRUD deposits impact on CIPS phenomenon, was described in this paper. The coupling among three essential physics, thermal-hydraulics, CRUD and neutronics described in the framework was implemented by using CFD software STAR-CCM+, developing CRUD module, and using the neutronics code DeCART. The coupling among these codes was implemented by exchanging data between them using intermediate exchange files. A typical 3 by 3 PWR fuel pin problem was solved under this framework and the results were presented. Time-dependent solutions were provided for a 12-month simulation, including CRUD deposits inventory and their distributions on fuel rods, boron hideout amount inside CRUD deposits, as well as power shape changing over time. The results clearly showed the power shape suppression in regions where CRUD deposits exist, which is a clear indication of CIPS phenomenon.

Key Words: CRUD, CFD, Neutronics, Coupling, DeCART, STAR-CCM+.

1. INTRODUCTION

The DOE Consortium for Advanced Simulation of Light Water Reactors (CASL) has established a mission to develop and apply modeling and simulation capabilities to address three critical areas of performance for nuclear power plants (NPPs): cost, reduction in amount of used nuclear fuel and safety [1]. All these three objectives can be achieved by power uprates, lifetime extension and higher burnup through predictive simulations. Key phenomena limiting the improvements of reactor performance, as well as several challenge problems have been defined to guide and measure the CASL progress. Among these challenge problems, CRUD is an important one which is the key to resolve the CRUD-Induced Power Shift (CIPS) and CRUD-Induced Localized Corrosion (CILC) issues.

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CRUD-Induced Power Shift (CIPS), formerly known as power axial offset anomaly (AOA), has long been realized in the industry from early 1970s. In late 1980s severe AOA issues were found in Callaway nuclear power plant and later in other plants [2]. It’s normally featured in an abnormal shift in axial and radial power distribution, however generally shifted toward the bottom of the core. There have been many researches to find the root cause of AOA and many models to predict AOA phenomenon. It is now generally accepted that AOA (or CIPS) is caused by neutron flux suppression in upper part of assemblies where large amounts of boron is held in the porous CRUD deposits on fuel pin surfaces. Three key factors were identified as root causes for CIPS phenomena, i.e., subcooled boiling on fuel rod surfaces, corrosion products in coolant, and soluble boron in coolant. In nuclear power plants, major corrosion products are produced from steam generator tubes, providing potential source for CRUD deposits. Subcooled boiling in the upper part of reactor core is the driving force to accelerate CRUD deposition on fuel rod surfaces. As CRUD deposits are formed, boron accumulates inside this porous layer and then affects the neutron flux shape.

The CIPS phenomenon shows a very complicated multi-physics nature. It involves the coupling between thermal-hydraulics, CRUD deposition, boron hideout inside CRUD deposits, and reactor physics. A lot of efforts have been devoted to understand these single mechanisms as well as the coupling effect between them. The relationship between boiling and deposition was studied by several researchers. Partridge [3] provided experimental evidence of ring-shaped deposition around bubbles, which led to the theory that deposition happens at the triple phase interface as bubbles grow. Disk-shaped deposits beneath bubbles, later revealed by Hospeti and Mesler [4], led to a different MEM (Micro-layer Evaporation Model) theory. Different theories [5, 6, and 7] were also proposed to explain the deposition of particulates due to bubble formation. In recent research, Hitesh [8] carried out an experimental study on the relationship between heterogeneous nucleate boiling and deposition of metallic colloidal particles for pool boiling conditions at atmospheric pressure. Hawkes [9] experimentally examined the CRUD deposition and boron hideout with typical PWR thermal-hydraulics and water chemical conditions.

Boron hideout, by itself, is also a multi-physics phenomenon, which involves complex coolant phase change within CRUD deposits, solute transport, and chemical reactions. MacBeth [10] was the first one to propose the wick boiling concept for boiling heat transfer within CRUD deposits. Cohen [11] later proposed a simple one-dimensional model to describe the heat transfer and solute mass transfer within a CRUD layer. Based on previous studies, Pan [12] proposed a two-dimensional wick boiling model, which simulates heat conduction, evaporation of coolant, solute convection and diffusion balance in CRUD deposits. In a recent study published by Henshaw et. al. [13], which is based on Cohen’s one-dimensional model, additional chemical reactions were taken into consideration in the model. The model is able to predict concentrations of chemical species, pH values, and local temperatures at different depths in CRUD deposits.

Efforts were also put into the examination and analysis of CRUD deposits from PWR fuel surfaces as well as CRUD deposits formed under PWR-like conditions. Purposes of such examinations were to identify geometry and chemistry characteristics of CRUD deposits, and also to find out in what kind of chemical form boron is captured in the CRUD. An original boron hideout theory was proposed that the CIPS is attributed to the precipitation of lithium metaborate ($\gamma$-LiBO$_2$) in the CRUD deposits [14]. Experimental work performed by Hawkes [9] examined...
the boron-bearing species deposited in prototypical CRUD grown under typical PWR reactor operating conditions. This boron-bearing species has been identified to be lithium tetraborate (Li2B4O7). Recent work done by Sawicki [15] examined the ~100-µm-thick deposits taken from the fuel assemblies after Cycle 9 in the Callaway nuclear power plant. A large amount (about 50 wt%) of Ni–Fe oxyborate (Ni2FeBO5, mineral name bonaccordite) was found in these deposits. All evidence indicates that, other than simple solute convection and diffusion, complicated chemical reactions and precipitation of certain species are also present in CRUD deposits. A few other approaches [16] have also been made to predict the CIPS phenomenon in a coupled manner.

2. MODEL DESCRIPTIONS

The work presented in this paper describes a framework for solving the coupled multi-physics problem, including subcooled boiling, CRUD growth, boron hideouts and reactor physics. This framework was implemented using three major modules: 1) Thermal-hydraulics module, which solves the conjugated heat transfer between fuel and coolant, as well as the subcooled boiling. This module is implemented by using the commercial CFD software, STAR-CCM+ [17]; 2) CRUD module predicts the CRUD growth rate, distribution on fuel surfaces, and boron hideouts, which was accomplished by developing a CRUD code; and 3) Neutronics module, which solves the neutron transport equation, was implemented by using the DeCART code [18,19]. The coupling between these codes is implemented by using intermediate exchange files [20], which is normally described as loose coupling.

The time-dependent coupling scheme is shown in Figure 1. The coupling scheme has three steps,

1) An inner coupling between the thermal-hydraulics and neutronics modules is first performed to determine power distribution and boiling conditions. Converge is reached as both power distribution calculated from DeCART and thermal-hydraulics conditions calculated from STAR-CCM+ are stable.
2) Assuming T/H conditions established in step 1 are stable for a period of time, e.g. one month, using the CRUD module to determine the accumulated CRUD thickness and boron hideout inside the CRUD.
3) As CRUD thickness, distribution, and boron hideout amount are obtained in step 2, update DeCART input file accordingly based on Step 2 results. March to the next time step, repeat steps 1 and 2.

2.1. Thermal-Hydraulics Model

The conjugated heat transfer is solved with the commercial CFD software, STAR-CCM+. The three-dimensional fuel pin geometry and mesh are prepared in Cubit [21] and Gambit [22]. For simulation of typical PWR fuel pins, spacers and mixing vanes are not included at the current stage due to the complexity of the grid spacer geometry and coupling between STAR-CCM+ and DeCART. The commonly used k-epsilon turbulence model is used to solve the coolant flow problem. An additional boiling model is used to predict the subcooled flow boiling behavior as fuel surface temperature exceeds the coolant saturation temperature. For subcooled boiling,
there are several correlations to use, such as Thom [23] and Jens-Lottes [24] correlations. The Thom correlation is

$$\Delta T_{sat} = 22.5 q''^{0.5} e^{-P/18.7}$$

(1)

where, $\Delta T_{sat}$ is wall superheat, in K; $q''$ is heat flux, in MW/m²; and $P$ is pressure, in MPa. The Jens-Lottes correlation is

$$\Delta T_{sat} = 25 q''^{0.25} e^{-P/62}$$

(2)

where, $q''$ is heat flux, in MW/m²; and $P$ is pressure, in bar.

Recent research [25] showed that the Thom correlation gives the best agreement with the nucleate boiling heat transfer test with typical PWR rod bundle conditions. The STAR-CCM+ boiling model, however, uses the Rohsenow’s [17, 26] nucleate boiling correlation shown in Eq. (3) to predict the surface heat flux due to boiling,

$$q'' = \mu_l h_{fs} \sqrt{\frac{g(\rho_l - \rho_v)}{\sigma}} \left( \frac{C_{p,l} \Delta T_{sat}}{C_{sf} h_{fs} Pr_l^{1.7}} \right)$$

(3)

where, $q''$ is heat flux; $\mu_l$, $C_{p,l}$, $\rho_l$, and $Pr_l$, are dynamic viscosity, specific heat, density and Prandtl number of the liquid phase; $g$ is gravity; $\sigma$ is surface tension; $h_{fs}$ is latent heat. All quantities are in SI unit. $C_{sf}$ is an empirical coefficient experimentally determined. To fit the Thom correlation, this coefficient was modified accordingly to have better accuracy.
The coupling between STAR-CCM+ and DeCART was implemented via temporary files. STAR-CCM+ reads in power densities provided from DeCART and outputs fluid/solid properties as input of DeCART.

### 2.2 CRUD Model

It is essential to predict CRUD deposits rate on fuel surfaces and their distributed along the full length fuel pin. However, there is no mechanism based predictive model which can be directly applied in this framework. A generally accepted assumption is that all corrosion products released from the steam generator tube surfaces and other structure surfaces will eventually deposit onto fuel surfaces, where the corrosion mass balance holds. Thus, the total CRUD inventory growth rates on the fuel rods can be determined by corrosion rates in the steam generators. For typical PWR’s, the corrosion products are mainly released from Alloy 600 and stainless steel surfaces [27], and correlations for these two corrosion rates per unit surface area are experimentally determined as,

\[
CR_{600} = 1.7 \times 10^6 \times [H^+] + 1.84 \text{ mg/dm}^2\text{-month} \tag{4}
\]

for Alloy 600, in which, \(CR_{600}\) is the corrosion rate of Alloy 600 and \([H^+]\) is the concentration of \(H^+\).

For stainless steel the corrosion rate, \(CR_{SS}\), is given as,

\[
CR_{SS} = 3.4 \times 10^6 \times [H^+] + 3.66 \text{ mg/dm}^2\text{-month} \tag{5}
\]

The total corrosion rate for each of these two materials can be calculated as the product of its corrosion rate per unit surface area and its total surface area. The total corrosion rate of a typical PWR system is the sum of corrosion rates of these two materials. Also, note equations (4) and (5) are for metal release rate, and since CRUD is normally in the forms of metal oxides, mass conversion ratios are needed to calculate CRUD deposits rate.

As the total CRUD deposition rates are obtained, the key is to determine the distribution on fuel rod surfaces. Localized subcooled boiling is generally considered as the driving force to accelerate CRUD deposition. In this model, it is assumed that the CRUD deposits only where subcooled boiling takes place, and the deposit amount is proportional to the local evaporation rate, i.e.,

\[
DR_{CRUD} \propto R_{evp} \tag{6}
\]

where, \(DR_{CRUD}\) is local CRUD deposition rate; and \(R_{evp}\) is local coolant evaporation rate. Therefore, the local CRUD deposition rate can be calculated as,

\[
DR_{CRUD,i} = \frac{R_{evp,i}}{R_{evp,\text{total}}} \cdot DR_{CRUD,\text{total}} \tag{7}
\]

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in which, subscript $i$ means the $i^{th}$ spatial region; and subscript total means the total amount within the system.

The boron hideout model is derived from Cohen’s one-dimensional work [11]. As both porous CRUD layer and boiling are present, soluble boron will flow with fluid into the porous layer driven by the coolant phase change taking place inside the layer. Boron concentration increases until a balance is reached between boron convection and boron back diffusion due to high concentration gradients inside the CRUD layer. The ratio of averaged boron concentration inside the CRUD layer to the bulk boron concentration is provided by Cohen [11] as,

$$
\bar{\bar{f}} = \frac{D_f \rho_L h_{fg}}{\delta q'' \left(1 - \frac{1}{\cosh(\alpha\delta)}\right)} \left[\exp\left(\frac{q'' \delta}{D_f \rho_L h_{fg}} \left(1 - \frac{1}{\cosh(\alpha\delta)}\right)\right) - 1\right]
$$

where, $D$ is diffusion constant for the soluble species; $f$ is surface area ratio not occupied by chimneys of CRUD deposits; $\alpha$ is a constant related to CRUD geometry and fluid thermal properties; $\delta$ is CRUD layer total thickness; $q''$ is surface heat flux; $\rho_L$ is coolant density; and $h_{fg}$ is latent heat of coolant.

### 2.3 Neutronics Model

The framework uses the DeCART code to solve the neutron transport problem. The DeCART (Deterministic Core Analysis based on Ray Tracing) code is a whole core neutron transport code capable of direct sub-pin level flux calculation at power generating conditions for either a PWR or BWR core [18,19]. This code employs a synthesis method of planar MOC (method of characteristics) and 1-D axial diffusion. A large amount of calculation time can be saved by employing this kind of synthesis method, since the 3-D MOC could be too time consuming. This code does not require an external mesh or cross-section generation tool as these features are built in, which simplifies efforts of user input.

A special module is also built into DeCART to couple with CFD, i.e., STAR-CCM+. It is capable of reading position info and fluid/solid properties, such as temperature and density, from a typical STAR-CCM+ output file. Depletion calculation was not included in the current work, but will be implemented in future work.

### 3. MODEL RESULTS

In this section, a typical 3 by 3 PWR fuel pin problem is solved under the framework and the results are presented. A schematic drawing of the geometry from the top view is shown in Figure 2. Typical PWR parameters are used for the geometry; the active length of a fuel pin is 3.865m. Spacers and mixing vanes were not included in the problem as explained in previous sections.
The 3-D geometry and mesh were created in Cubit [21] and Gambit [22]. Effort was made to create the mesh with pure hexagonal cells. The mesh contains 0.58 million hexagonal cells and 1.6 million faces. The original mesh created in Cubit and Gambit, as well as after it is read into STAR-CCM+, is shown in Figure 3. The mesh was created relatively coarse in axial direction while much finer in radial direction. This is an approach to reduce the overall mesh cell number while still keeping reasonably good accuracy, since the temperature gradient is much higher in the radial direction than it is in the axial direction.

Figure 2. Schematic drawing of the 3 by 3 PWR fuel pin problem

Figure 3. Mesh generated with Cubit [21] and Gambit [22] (left), and mesh read into STAR-CCM+ [17] (right)
Figure 4. A typical 3 by 3 PWR fuel pin input for DeCART (left) and a special pin with CRUD layer (right)

For the DeCART input, the 3.865m-long-active-length fuel was divided into 20 equal axial planes. For the initial state (time = 0), when there is no CRUD deposits on clad surfaces, a pin has a regular layout including pellet, cladding, and moderator. As CRUD deposits on cladding surface, an additional CRUD region is added to the surface of the fuel pin, reflecting the thickness of the CRUD layer and boron inventory held in the CRUD layer. Both of these two numbers were prepared from the CRUD module. The CRUD model has the same axial resolution as the CFD mesh, both of which are much finer than the axial resolution used in neutronics calculation. Therefore, both CRUD thickness and boron concentrations were averaged locally for the DeCART input. A typical DeCART input is shown in Figure 4, in which both the 3 by 3 geometry and a single pin with CRUD layer are presented.

The simulation was performed with a total time length of 12 months and a time step of 2 months. As described previously, in each time step, an inner loop between STAR-CCM+ and DeCART was performed to converge the power and T/H solutions. The CRUD deposition rate and distribution were then calculated from the CRUD module assuming constant conditions over the time step. Figure 5 shows the CRUD deposition history for a 12 months simulation. It can be noted that the growth of the CRUD layer is nearly linear with time. This is based on the assumption that the coolant pH value during the simulation was fixed and therefore the corrosion source term is constant. The change in CRUD thickness from 10th month to 12th month in the region between 160 cm to around 180 cm shows a different behavior than other time steps. This is caused by a reduced local heat flux due to the power suppression as a result of CIPS phenomenon, which is shown later in Figure 7. Figure 6 shows the boron hideout amount history during the 12 month simulation. The boron hideout rate shows a faster increasing trend over time than the CRUD deposition rate. As shown in equation (8), the boron hideout rate has an exponential relationship with CRUD thickness, which is the result of balance between boron diffusion and convection. As CRUD deposits grow linearly with time, the boron concentration increases nearly exponentially. This exponential relationship also explains why, in general, there is no CIPS observed for most PWR reactors which typically have around 25 microns thick CRUD.
CRUD deposits in the subcooled boiling regions. However, severe CIPS is generally exhibited by reactors where the CRUD thickness reaches ~100 microns. The power shape history, shown in Figure 7, also indicates the same trend. Comparing the power shape in the first 6 months of time period, the power shape did not show significant changes over time. After the 6th month, in regions where CRUD deposits have formed, local power starts to reduce as a result of neutron flux suppression, which is a clear sign of CIPS phenomenon.

![CRUD Thickness History](image1)

**Figure 5. CRUD thickness history for a 12 months simulation**

![Boron Hideout History](image2)

**Figure 6. Boron hideout history for a 12 months simulation**
4. CONCLUSIONS

In this study, a coupling framework was described which is able to simulate the CRUD deposition and CIPS phenomenon. This framework includes three essential physics, thermal-hydraulics, CRUD and neutronics, which are implemented by using the CFD software STAR-CCM+, developing CRUD codes, and using the neutronics code DeCART. The coupling between these codes was implemented by exchanging data between these codes using intermediate exchange files. A typical 3 by 3 PWR fuel pin problem was solved under this framework without depletion calculation. The results clearly showed the power shape suppression in regions where CRUD deposits exist, which is an indication of CIPS phenomenon. This framework, however, is still in its initial development stage. Additional work needs to be done to improve the framework, e.g., applying and developing higher accuracy and mechanism based models, including depletions, verification and validation on single models and the framework.

![Figure 7. Power shape history for a 12 months simulation](image-url)
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