High-Fidelity Simulation of CRUD Deposition on a PRW Fuel Pin with Grid Spacers: A Proof–Of-Principle Using The Fully-Coupled MAMBA/DECART/STAR-CCM+ Code

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May 12-17, 2013:

CASL-U-2013-0097-000
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ABSTRACT

The operational issues that arise due to CRUD (Chalk River Unidentified Deposit) build-up on PWR fuel pins include CRUD induced power shift (CIPS) and CRUD induced localized corrosion (CILC). These phenomena lead to reduced operating margin and compromised fuel rods. The work presented here develops a framework for the high-fidelity simulation of CRUD deposition. This framework includes three primary physics of neutronics (DeCART), thermal-hydraulics (STAR-CCM+) and CRUD chemistry (MAMBA), and the prominent feedback mechanisms between each of the physics. A fully-coupled simulation of a pressurized water reactor fuel pin cell with 3.3 wt% enriched uranium dioxide fuel was performed over a cycle length of 500 effective full-power days. The simulation recreated the classic “striped” CRUD pattern often seen on pulled fuel rods containing CRUD. It is concluded that striping is caused by the flow swirl induced by grid mixing vanes. The flow swirl yields large azimuthal temperature variation, which impacts the locations where CRUD deposits. Conversely, the flow swirl is correlated to increased shear stress along the cladding surface and subsequent erosion of the CRUD layer. The CIPS condition of the core is concluded to be primarily controlled by lithium tetraborate precipitation. This precipitation occurs when soluble boron and lithium species reach their solubility limit within the CRUD layer, where localized subcooled nucleate boiling has occurred. A localized reduction in power occurs due to high neutron absorption cross section of boron-10. The depletion simulation shows that, at a core burnup of 31.363 GWD/MTU, 6.13 g of nickel ferrite and 13.38 mg of boron were deposited within a CRUD layer that reached a maximum thickness of 95 μm. This amount of CRUD deposition caused a maximum axial offset of the power distribution of -7.2% at a burnup of 22.5 GWD/MTU, or 360 effective full-power days. The operating effects due to this magnitude of CRUD build-up and power shift may include mandatory reduction of power, fuel leaks, or plant shutdown.
1. INTRODUCTION

CRUD induced power shift (CIPS), historically known as axial offset (AO), is an important phenomenon that requires careful risk assessment. The risk for CIPS increases with power uprates and longer cycles due to the increased potential for thicker CRUD deposits. CIPS originates from an axially asymmetric boron deposit which resides in the CRUD layer that coats the surfaces of the fuel rods. The CRUD deposit is typically thicker on the upper regions of the fuel rods due to the higher temperature of the surrounding coolant and increased probability of subcooled nucleate boiling (SNB) [1]. Accurate modeling of the phenomena involved in CRUD deposition requires the use of high-fidelity, multi-physics simulations. Specifically, the turbulence induced by the mixing vanes and the location of the hot spots along the cladding surface cannot be captured in current subchannel codes. Therefore, within this framework, three computational tools are used: (1) DeCART for the full-core neutron transport, (2) STAR-CCM+ for the computational fluid dynamics (CFD), and (3) MAMBA for the macro-scale coolant chemistry and CRUD deposition.

1.1 Physics of CRUD Deposition in PWRs

In pressurized water reactors (PWRs), the primary CRUD source is corrosion of the steam generator tubing, and it develops as oxygen diffuses into the base metal and the alloy elements are transformed from the metallic state to the oxide state. Divalent metal ions are then released into the water as soluble metal ions [2]. The metal ion release rate is dependent on the diffusion coefficient of oxygen, the oxide thickness and composition, and the concentration of the metal already in the coolant, among other contributors [3]. The corrosion particulates circulate the primary loop and deposit on the fuel rods. These CRUD deposits are composed mostly of nickel ferrite (NiFe$_2$O$_4$), nickel oxide, and nickel metal with other nickel-iron-chrome spinels [4]. The boron concentration within the CRUD layer increases with increasing CRUD thickness due to the higher cladding temperatures and increased internal boiling within the CRUD layer. The internal boiling occurs within “chimneys” that develop in the CRUD, as shown in Figure 1. The coolant and its soluble species, such as boric acid and lithium, are drawn in. As the coolant vaporizes, the soluble species are left behind and concentrate along the cladding surface. The subsequent precipitation of lithium tetraborate is governed by equilibrium thermodynamics. It is a function of temperature and determined experimentally.

Figure 1 – Sample CRUD layer showing in-flow of water and out-flow of steam in chimneys leading to (Li$_2$B$_4$O$_7$) precipitation (left) [5], and the heat transfer within a chimney (right) [4].
1.2 Feedback Mechanisms

Modeling of CRUD deposition requires the prediction of axial and azimuthal distributions of power and cladding temperature, as well as the modeling of the flow swirling induced by the grid spacers. Furthermore, modeling of CRUD erosion also requires detailed information about the local turbulent kinetic energy (TKE) or shear stresses at the cladding surface.

The presence of hot spots on the cladding surface triggers the deposition of CRUD, which yields an increase in the thermal resistance between the cladding and coolant. This leads to an increase in the cladding temperature at the location where CRUD is depositing, causing more CRUD deposition at the same location. This is a positive feedback mechanism. Conversely, the neutronics provides a negative feedback. Because of the neutron absorbers present in the CRUD—primarily boron and secondarily nickel ferrite—the deposition of CRUD on the cladding surface yields a local decrease in the power. A decrease in the local power will lead to a decrease in the local cladding temperature and to less CRUD formation. An additional thermal-hydraulic feedback is caused by shear stress, or turbulent kinetic energy near the cladding surface. TKE is positively correlated to the erosion of the CRUD layer. Moreover, convective heat transfer improves between the cladding and coolant with increasing TKE, which leads to less CRUD deposition. Therefore, CRUD erosion is high at locations where CRUD deposition is generally low. The combination of these two positive thermal-hydraulic feedback mechanisms have a strong contribution to the classic striping patterns of CRUD observed downstream from grid spacers.

1.3 Coupling Strategy

A coupling strategy between DeCART (neutronics), STAR-CCM+ (thermal-hydraulics) and MAMBA (CRUD chemistry) was developed using a sequence of three separate, two-way coupling interfaces as shown in Figure 2 (left). The transfer of data between the three physics occurs by automated file exchanges. A driver code developed for the framework allows the depletion cycle to be simulated continuously and without additional user support.

In the neutronics/CFD coupling interface, DeCART provides STAR-CCM+ with the volumetric heat source in the fuel pin for each CFD mesh, while STAR-CCM+ supplies DeCART with fuel temperature and fluid density distributions for each DeCART mesh. This coupling interface has previously been implemented and demonstrated [6]. During the depletion, the temperatures and power densities are exchanged and iterated until converged. In the CFD/CRUD coupling interface, STAR-CCM+ provides MAMBA with the heat flux, the TKE near the cladding, the cladding wall temperature, and the fluid temperature distributions. MAMBA provides STAR-CCM+ the additional thermal resistance between the cladding and fluid introduced by the CRUD formation on the cladding surface. The CRUD thermal resistance is a function of the thickness of the CRUD layer and the CRUD thermal conductivity. The accumulation of a CRUD layer on the cladding surface also influences the wall roughness, which is not accounted for in the current investigation. In the CRUD/neutronics coupling interface, MAMBA provides DeCART the boron-10 concentration in the CRUD, the CRUD thickness and CRUD concentration in the form of NiFe₂O₄. The boron destruction rate is passed form DeCART to MAMBA to capture the reduction of the boron in the CRUD due to the neutron flux. Figure 2 also shows the corrosion source term provided by BOA (Boron-Induced Offset Anomaly), a code developed by EPRI.
Figure 2 – Data exchange between the primary physics (left), and time stepping scheme (right).

Figure 2 (right) illustrates the temporal updates between the three codes. The DeCART/STAR-CCM+ time stepping scheme consists of a fixed-point Gauss-Seidel iteration. At each iteration, DeCART updates the power distribution on the basis of the fuel temperature and coolant density distributions computed by STAR-CCM+. Next, the STAR-CCM+ solution is updated based on the power distribution supplied by DeCART. The iterations continue until the convergence criteria are satisfied for time = t₀ days. Next, the cladding temperature, heat flux and TKE near the cladding wall is passed to MAMBA. Then, MAMBA calculates the CRUD formation to t₀ + t_step days. In the following DeCART depletion calculation, the CRUD constituent concentrations at t₀ + t_half_step and t₀ + t_step days are used. The results presented in Section 4 use t_step = 4 days for the first 20 days and then t_step = 20 days for the remaining cycle.

2. COMPUTATIONAL TOOLS DESCRIPTION

DeCART (Deterministic Core Analysis based on Ray Tracing) is a whole core neutron transport code capable of direct sub-pin level flux calculation at power generating conditions of a light water reactor (LWR). It requires neither a priori homogenization nor group condensation as needed in conventional reactor physics calculations. DeCART solves the three-dimensional neutron transport problem employing a 2D-1D method in which the planar solution is performed using the Method of Characteristics (MOC) solutions and the axial solution is performed using the Nodal Expansion Method (NEM) based kernel. The depletion calculation is performed using the predictor/corrector method and is well validated for a wide range of LWR applications [7].

STAR-CCM+ is a commercial computational fluid dynamics (CFD) code that solves the balance equations for continuity, 3-D momentum, and fluid enthalpy on a very fine 3-D mesh. STAR-CCM+ is capable of modeling conjugate heat transfer, such that the conduction process is modeled within the fuel pellet and cladding and the convective heat transfer is modeled in the cooling fluid that surrounds the pin. The Reynolds-Averaged Navier-Stokes (RANS) approach for the solution of the k-ε transport equations was used for the turbulence modeling. The Two-Layer All y+ model was used for the wall treatment.

MAMBA (MPO Advanced Model for Boron Analysis) v2.1 simulates 3-D CRUD growth along the surface of a single fuel rod. The primary physics and chemistry associated with CRUD
formation currently treated in MAMBA include: (1) solving a general non-linear 3D heat transport equation for the CRUD layer including localized heat sinks due to internal boiling within the CRUD layer, (2) an adaptive grid which grows radially in time as mass deposits on the surface of the CRUD, (3) time evolving microstructure (porosity) of the CRUD layer due to localized deposition and precipitation of nickel ferrite and lithium tetraborate within the pores of the CRUD, (4) time evolving lithium and boric acid coolant chemistry both at the CRUD surface and inside the pores of the CRUD, (5) mass transport of various soluble coolant species into the interior of the CRUD due to boiling induced Darcy flow, (6) diffusion of various soluble species inside the CRUD due to the flow induced concentration gradients within the CRUD layer, and (7) mass evaporation in the form of steam vapor due to the localized boiling inside the CRUD layer. The CRUD erosion based on the TKE is calibrated on a qualitative basis to best match observed CRUD build-up. Erosion kinetics within MAMBA will be implemented in the future.

3. SIMULATION MODELS

3.1 DeCART

The DeCART pin cell model consists of a 3-D pin with an active fuel height of 365.76 cm and 20 cm thick water reflectors at each end. The radial boundary conditions are reflective, while the axial boundary conditions are vacuum. The power of the fuel pin is 107.17 kW, which corresponds to a peaking factor of about 1.6 for a pin from a typical 17x17 PWR fuel assembly. Eight 4 cm tall grid spacers with 0.24 mm thick walls are included to simulate the neutron absorption effects. The fuel composition is uranium dioxide (UO$_2$) with 3.3 wt% enriched uranium-235. The cladding and grid spacer material is Zircaloy-2 and no fuel-cladding gap is modeled. The coolant boron concentration (CBC) is letdown during depletion from 1950 ppm to 10 ppm; the letdown shape and magnitude was tailored for the pin cell model to maintain realistic core parameters such as the moderator temperature coefficient. Figure 3 shows the pin cell geometry with select grid spacers and all flat source regions explicitly shown: 48 within the fuel and 16 within each the cladding, CRUD, moderator, and grid spacer regions. The outermost radial region is initially filled with moderator and is reserved for CRUD, which is “deposited” after input processing. The CRUD deposition is azimuthally dependent, allowing the CRUD concentration to vary circumferentially around the rod. When CRUD is deposited, the coolant is displaced and the remaining mixture is homogenized within a user-defined 200 μm thick region.

Figure 3 – DeCART pin cell model with explicit mesh (left), zoom view of azimuthally-dependent CRUD concentration (middle), and geometry of grid spacers (right).
3.2 STAR-CCM+

The CFD domain includes the solid structure containing the fuel pellet and cladding, the water domain in the subchannel surrounding the fuel pin, and the grid spacers. An inlet velocity of 5.278 m/s and pressure boundary condition is imposed for the inlet and outlet axial planes of the coolant domain, respectively. Symmetric boundary conditions are imposed on the lateral surfaces of the water domain. No-slip conditions are imposed on the grid spacers, pin walls and on the cladding surface. A volumetric power source is used in the fuel domain (provided by DeCART). The coolant density was calculated according to the following third-order polynomial: \( \rho(T) = -0.0000116905 \cdot T^3 + 0.01225 \cdot T^2 - 4.84697 \cdot T + 1670.3259 \). The inlet temperature is 556.76 K, and the system pressure is 15.51 MPa. The UO\(_2\) fuel and cladding thermal conductivity are set constant at 6 and 17 W/m-K, respectively. In the future, the fuel conductivity will be dependent on temperature. The fluid-dynamic simulation includes conjugate heat transfer for the calculation of the temperature distribution in the fuel and cladding domains. The CFD domain was meshed by means of polyhedral cells. Three explicit grid spacers including four mixing vanes, as shown in Figure 4 (left), are modeled. The five other spacers were not modeled to reduce computation time. The grid spacer regions, which rest at 203.28 cm, 249.00 cm, and 294.72 cm from the bottom of the active fuel, were discretized using polyhedral cells together with three layers of prismatic cells at the wall. The computational mesh upstream and downstream of grid spacers was generated by extrusion, applying the hyperbolic tangent law. Approximately 1.6 million cells makeup this model. The convergence criteria were fixed at 1x10\(^{-6}\) for continuity, momentum, and energy. Figure 4 (right) shows the boundary conditions imposed and the cross section mesh.

![Figure 4 – STAR-CCM+ model showing grid spacer with mixing vanes (left), and boundary conditions and mesh (right).](image)

3.3 MAMBA

The MAMBA model consists of the same single pin cell geometry as previously discussed. The radial mesh of the CRUD region (between the cladding surface and the 200 µm boundary) adapts to the CRUD growth in 5 µm increments, with 40 radial mesh regions possible in this model. The azimuthal mesh consists of 16 uniform regions, aligning with the DeCART mesh. The pin is axially discretized into 74 uniform regions of 5 cm. The CRUD parameters include a user-defined initial porosity of 0.7 (which evolves in time), solid density of 5.33 g/cm\(^3\), a chimney radius of 4 µm, chimney density of 1.6x10\(^5\) #/cm\(^2\), and a chimney heat transfer coefficient of 2.12x10\(^6\) W/m\(^2\)K. The nickel ferrite surface deposition rate is given by an Arrhenius rate expression, \( k = A \exp[-E/RT] \), where \( A = 110.0 \text{ cm/s} \) and \( E = 10 \text{ kcal/mole} \). The CRUD growth rate multiplier due to SNB is set to 1.5x10\(^{-3}\) cm\(^3\)/J. The coolant species concentrations
are also fixed for soluble nickel, soluble iron, and particulate NiFe$_2$O$_4$ as 0.22 ppb, 1.32 ppb, and 1.76 ppb, respectively. The same CBC letdown as described for the DeCART model is imposed.

4. FULLY-COUPLED DEPLETION RESULTS

4.1 Converged Steady State Solution (0 days)

Prior to depletion and CRUD deposition, the converged solution at zero burnup is found by a coupled DeCART/STAR-CCM+ simulation. The first iteration of the initial convergence of neutronics and thermal-hydraulics begins with a single steady state DeCART solution followed by about 800 STAR iterations using the provided power distribution, at which the convergence criteria for continuity, momentum, and energy are met. This iteration scheme continues for 4 total iterations and the final core characteristics are an effective multiplication factor of 1.13099 and an axial offset of +4.15%: This is the starting point for the 500-day depletion simulation. The radially-integrated, converged axial power distribution (left) and average CRUD region temperature distribution (right) are shown in Figure 5. The locations of the eight grid spacers in DeCART, and the associated power depressions due to the increased neutron absorption by the grid material, are labelled with arrows. The purple, bolded arrows represent the locations of the three explicitly modeled grid spacers and mixing vanes within the STAR-CCM+ model. The average CRUD region temperature, which is initially filled with coolant, increases approximately 50 K in Figure 5. The substantial increase in heat removal due to the increase in turbulent mixing immediately following the three explicit grid spacers with mixing vanes is demonstrated.

![Figure 5 – Converged DeCART/STAR axial power distribution with grid spacers (left), and average CRUD region temperature (right).](image)

4.2 Fully-Coupled CRUD Deposition

The integral CRUD mass, maximum thickness and integral boron mass along the rod during the cycle depletion are shown in Figure 6. Between 200 and 400 effective full-power days (EFPD), the boron within the CRUD layer quickly increases due to the precipitation of lithium tetraborate. After 400 EFPD, the boron mass decreases due to diffusion of species and reduced CBC feeding the CRUD layer. The boron density within the CRUD layer is shown in Figure 7.
(right), and it is seen that the precipitation occurs locally in three or four segregated areas. The precipitation threshold of the concentration of the boric acid and lithium within the coolant is exceeded at these locations. This is attributed to local SNB that pulls coolant into the CRUD and to the cladding surface, concentrating the boric acid and lithium species during vaporization. Once \( \text{Li}_2\text{B}_4\text{O}_7 \) precipitation occurs, the dense boron creates a localized neutron sink, which jointly reduces the power and temperature of the cladding surface. The effect of the grid spacer mixing vanes on the CRUD build-up is also evident in Figure 7; the high TKE and associated wall shear stress following the vanes erode the CRUD layer nearly down to the cladding.

Figure 6 – Integral CRUD mass, max thickness and integral boron mass during the cycle.

Figure 7 – TKE near the clad surface (left), boron density within CRUD layer (mg/cm\(^3\)) along length of the fuel rod at 100 (left), 300 (middle), and 500 (right) EFPD – note color bar scales.

Figure 8 (left) shows the evolution of the cladding temperature for three burnup states: 100, 300, and 500 EFPD. As the CRUD thickens along the upper regions of the fuel pin cladding, heat transfer from the solid rod to the coolant deteriorates, leading to local rises in the temperatures.
Consequently, the possibility of SNB increases as does the likelihood of CILC and fuel failure. Figure 8 (right) shows the TKE (top) and the cladding wall temperature (bottom) in the vicinity of the second grid spacer. Both the TKE and temperature present a characteristic striped pattern due to the flow swirl that the mixing vanes induce around the rod. As expected, these properties are anti-correlated, where an increase in TKE increases the convective heat transfer leading to a decrease in temperature. Consequently, the CRUD deposition and boron hideout follow a similar striping pattern as shown in Figure 9.

![Figure 8](image1.png)

**Figure 8** – Temperature (°C) in CRUD layer along rod at 100 (left), 300 (middle), and 500 (right) EFPD, and TKE (right-top) and clad temperature (right-bottom) near spacer 2 at 300 EFPD.

![Figure 9](image2.png)

**Figure 9** – CRUD thickness and boron surface density along length of fuel rod at 100 (left), 300 (middle), and 500 (right) EFPD.

Maintaining sufficient operating margins according to the Nuclear Regulatory Commission (NRC) guidelines is a primary concern of the operating utility. CRUD build-up alters the power
distribution within the reactor core from the expected. The evolution of the axial power profile with cycle depletion for the coupled DeCART/STAR-CCM+ (no CRUD) simulation and the fully-coupled MAMBA/DeCART/STAR-CCM+ simulation are shown in Figure 10 and Figure 11, respectively, for three burnup states: 6.27, 18.82, and 31.36 GWD/MTU. Without CRUD deposition, the expected “double-hump” power distribution evolves. Comparison of the no CRUD and CRUD cases reveal clear differences by 300 EFPD, where localized reductions in power are seen in the upper regions—locations of lithium tetraborate precipitation. The dense boron-10 in the precipitate pushes the power distribution toward the bottom of the core. Fuel burnup favors the bottom-peaked core power and works to flatten the distribution by the end of cycle (EOC). However, the local power depression near a core elevation of 310 cm still exists.

Figure 10 – Axial power distribution for the coupled DeCART/STAR-CCM+ simulation at 100 (left), 300 (middle), and 500 (right) EFPD.

Figure 11 – Axial power distribution for the fully-coupled MAMBA/DeCART/STAR-CCM+ CRUD simulation at 100 (left), 300 (middle), and 500 (right) EFPD.

Figure 12 displays the difference in power at each axial elevation between the no CRUD and CRUD simulations. Generally, a power reduction occurs in regions of CRUD deposition, and a subsequent power increase occurs in the less affected regions. Because these plots show differences in relative pin powers, a decrease in power in one region must be balanced by an increase in another. The power shift caused by CRUD build-up and boron hideout causes nearly a 15% difference in relative powers near 310 cm elevation. By 500 EFPD, the localized effects of the diffusion of species out of the CRUD and the boron destruction are visible.
The CIPS condition is a core-wide (global) phenomenon and the axial offset of the power is strongly dependent on core characteristics such as moderator temperature coefficient, coolant boron concentration, and fuel enrichment. Therefore, realistic modeling of a single radially reflective fuel pin is challenging without the presence of burnable absorbers, burned fuel, etc. Nonetheless, the AO, which is calculated as the ratio of the difference between the integrated power in the top and bottom halves of the core and the sum of these integrated powers, is shown in Figure 13. Smaller time steps are taken at the beginning of cycle to capture the xenon build-up effects. The small amount of CRUD deposition, completely in the form of nickel ferrite, in the first several GWD/MTU leads to a slightly more negative AO than the no CRUD case. However, this difference is slight and varies due to the CBC. Once lithium tetraborate precipitation occurs (beginning around 12 GWD/MTU), a negative power shift begins. By a core burnup of 22 GWD/MTU, the AO magnitude reaches its maximum of 7.2%. A combination of the reduction of the CBC, diffusion of species out of the CRUD layer, boron destruction, and increased burn in the lower regions, lead to a net reduction in the boron hideout and a more positive AO by EOC.

Figure 13 – Axial offset of power distribution for no CRUD and CRUD simulations.

5. CONCLUSIONS & FUTURE WORK

Data reported by EPRI suggests a core average boron build-up of 0.005 pounds (2,267.96 mg) per assembly corresponds to a 5% AO difference [3]. The 13.38 mg of boron predicted at 360 EFPD in this fully-coupled simulation, extrapolated to a 17x17 assembly (assuming equal CRUD loading), gives 0.0085 pounds (3,866.8 mg). The difference in the axial offset predicted in Figure
13 is approximately 6%, which is proportionally comparable to the expected AO according to EPRI [3]. This comparison supports the global rate of CRUD growth and boron hideout is within expectation. Therefore, modeling a single radially reflective pin cell demonstrates the capability of the coupling framework and provides a basis for additional investigations of the physics and modeling parameters. A STAR-CCM+/MAMBA study focused on the thermal-hydraulic effects on CRUD deposition in a 4x4 pin cell array is presented in a companion paper [8]. A similar 4x4 pin array that features a water rod and fuel pin with an IFBA (integral fuel burnable absorber) layer is targeted for the next fully-coupled depletion simulation. The geometry in Figure 14 aims to demonstrate azimuthal heterogeneity and allow further understanding of the coupled physics.

![Figure 14 – 4x4 pin cell array featuring a water rod and a fuel pin with IFBA layer.](image)

6. **ACKNOWLEDGEMENTS**

This work was supported by an NRC fellowship, NRC faculty development grant NRC-HQ-11-G-38-0038, and the Consortium for Advanced Simulation of Light Water Reactors (www.casl.gov), an Energy Innovation Hub (http://www.energy.gov/hubs) for Modeling and Simulation of Nuclear Reactors under U.S. Department of Energy Contract No. DE-AC05-00OR22725.

7. **REFERENCES**


