

High-Resolution Multiphysics Analysis of CRUD Effects in Reactor Assemblies

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This study develops a high-fidelity multiphysics coupling framework to systematically investigate the impact of Chalk River unidentified deposits (CRUD) on pressurized-water-reactor (PWR) assemblies, integrating neutronics, thermal hydraulics, and chemical kinetics modeling. CRUD, formed via subcooled nucleate boiling (SNB) and corrosion-product deposition, alters local boron concentrations, thereby inducing a power shift (CIPS) due to CRUD and generating asymmetric axial power distributions. The proposed framework adopts an internally coupled approach, utilizing Picard iteration and a background-mesh technique to resolve multiscale computational challenges while maintaining numerical accuracy and efficiency. Numerical simulations of a 17×17 PWR fuel assembly reveal that CRUD deposition reduces the eigenvalue by 293 percent mille (pcm) and shifts the axial power peak downward by 21 cm, corresponding to a 6.27% axial offset. Radially, the effect of CRUD on power distribution remains minimal (approximately 0.04%). A critical observation is the dominant influence of surface heat flux on CRUD growth, with thicker deposits and elevated boron concentrations observed in high-power regions. CRUD-induced perturbations also exhibit a “neighboring phenomenon,” wherein CRUD-free fuel rods experience comparable axial power shifts due to neutron-flux disturbances. These findings underscore the intricate coupling between power distribution, SNB, and CRUD chemistry, providing valuable insights for enhancing reactor performance and safety.

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I. INTRODUCTION

Nuclear energy provides stable large-scale electricity generation while emitting substantially lower carbon emissions than fossil-fuel-based systems, offering a practical solution for reducing dependence on nonrenewable energy sources [1]. As a sustainable-energy option, nuclear power derives its advantages from exceptional energy density and significant greenhouse-gas mitigation capabilities [2–5]. Pressurized-water reactors (PWRs) represent the most prevalent technology in modern nuclear-energy systems, comprising more than 60% of operational reactors worldwide [6]. This dominance stems from the

well-established safety record, standardized designs, and efficient utilization of light-water coolant technology. Maintaining the safe and efficient operation of PWRs remains a critical challenge in contemporary nuclear-energy infrastructure [7]. Technological advancements in PWRs have significantly enhanced operational power levels and extended cycle durations. However, numerous PWR nuclear power plants have reported the accumulation of chemical deposits and corrosion products in fuel assemblies under prolonged operation and high-power conditions [8–10].

These anomalies, known as Chalk River unidentified deposits (CRUD) [11,12], were first identified in the 345-MWe German-designed KWU. Obrigheim PWR [13]. The formation of CRUD is depicted in Fig. 1(a). As the coolant flows upward through the reactor core, the heat-transfer mechanism on fuel cladding surfaces transitions from convective heat transfer to subcooled nucleate boiling (SNB) [14–16]. This transition represents a highly efficient mode of thermal-energy transfer. It facilitates the accelerated deposition of corrosion products circulating in the

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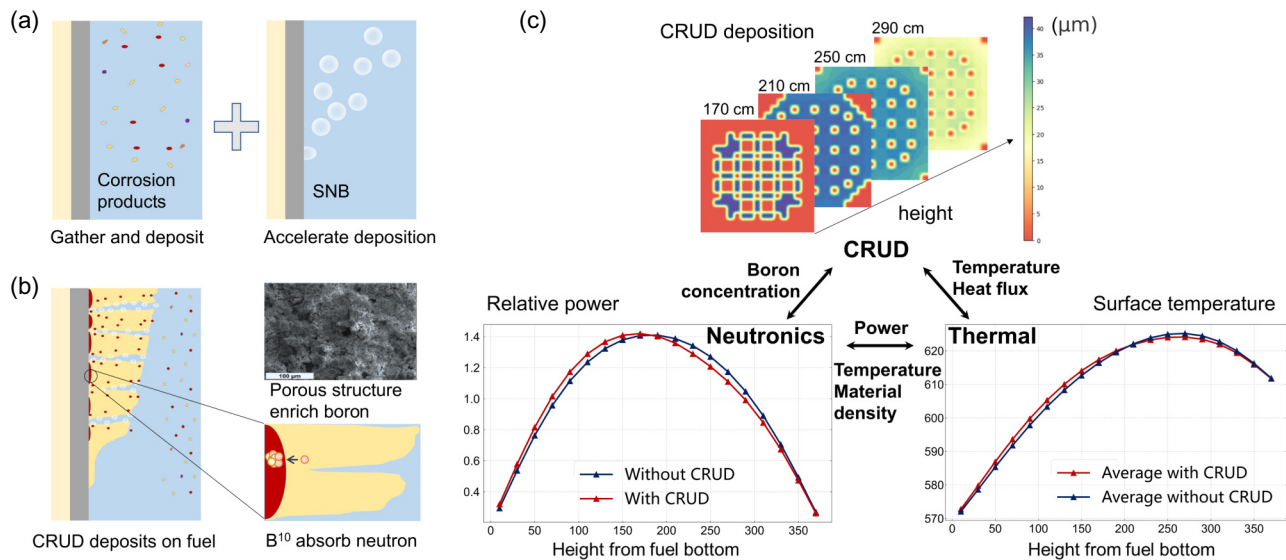


FIG. 1. The formation mechanisms, distribution, and effects of Chalk River unidentified deposits (CRUD). (a) The primary mechanisms of CRUD formation: subcooled nucleate boiling (SNB) accelerates the deposition of corrosion products in the coolant on the cladding surface. (b) The porous structure of CRUD deposits on fuel surfaces, demonstrating the boron-hideout capacity. (c) The CRUD-induced power shift (CIPS) resulting from boron-concentration effects within CRUD layers and other multiphysics interactions.

reactor coolant onto cladding surfaces, resulting in CRUD formation [17,18]. In Fig. 1(b), we show that CRUD primarily forms a porous layer adhering to cladding surfaces. The layer consists predominantly of nickel ferrite, nickel oxide, and metallic nickel, as well as other nickel-iron-chromium spinel compounds [12,19–22]. These deposits can further alter the local chemical environment, affecting the concentrations of elements such as boron and lithium [23,24].

Boron, primarily in the form of boric acid (H_3BO_3), serves as the principal additive in the primary coolant loop. It facilitates chemical control of reactivity through neutron absorption [25]. Being a highly effective neutron absorber in the coolant, the local enrichment influences the local neutron-flux distribution. It also promotes CRUD deposition via the formation of compounds such as $\text{Li}_2\text{B}_4\text{O}_7$ [26]. In Figs. 1(b) and 1(c), we demonstrate how the local accumulation of boron within the CRUD layer can induce abnormal axial power-distribution shifts in the reactor core. This phenomenon is known as CRUD-induced power shift (CIPS) [27,28], typically manifesting as significantly higher power levels at the bottom relative to the top. The accumulation of CRUD within fuel assemblies substantially reduces energy efficiency by impairing heat transfer and inducing neutron-flux distortions, which arise from the coupled interactions among corrosion chemistry, thermal hydraulics, and neutronics.

The computational analysis of CRUD deposition has been enabled by parallel developments in specialized simulation tools and multiphysics coupling strategies. Three complementary categories of computational tools

have emerged. Industry-developed codes such as Westinghouse’s boron-induced offset anomaly (BOA) [29,30] provide targeted solutions for boron-deposition analysis in operational reactors. Collaborative platforms such as MAMBA, from the Consortium for the Advanced Simulation of Light Water Reactors (CASL) [28,31–33] integrate materials-behavior and boron-transport modeling through multi-institutional efforts. Academic frameworks including the BOTANI multiphysics model from the Korea Advanced Institute of Science and Technology (KAIST) [34] and the CRUD code from the Shanghai Jiao Tong University (SJTU) [35] offer specialized capabilities for investigating fundamental chemical-transport mechanisms under various reactor conditions.

Current coupling approaches reflect progressively comprehensive simulation scopes. Component-scale frameworks established by the University of Michigan team have demonstrated the feasibility of integrating neutronics (DeCART [36]), fluid dynamics (STAR-CCM+), and CRUD chemistry (MAMBA) for single-pin [32] and three-pin [28] simulations. Plant-condition models developed at KAIST have incorporated actual PWR operating parameters to reproduce CRUD deposition patterns observed in operating reactors [34]. High-fidelity systems such as SJTU’s OpenMC-Fluent-CRUD coupling now enable full-scale fuel-rod analysis with Monte Carlo precision [35].

In this work, we introduce an internally coupled computational framework integrating multiphysics processes across spatial scales, from particulate deposition to assembly-level feedback, to enable precise feedback of CRUD effects on neutronics modeling. A 17×17

PWR fuel assembly is simulated to perform a comprehensive coupling analysis, yielding critical insights into the impact of CRUD after 180 days of steady-state operation. Our results reveal three key findings. First, we quantify the CRUD-induced power shift caused by boron deposition. Second, we characterize distinct spatial-deposition patterns along axial and radial directions. Third, we identify the dominant thermal-hydraulic and chemical mechanisms driving CRUD formation. These insights provide a systematic understanding of the coupled neutronics, thermal hydraulics, and chemical interactions governing CRUD behavior. The structure of the paper is organized as follows. Section II details the computational framework, including the neutronics, thermal hydraulics, and CRUD models used in the coupled simulations. This section explains the fundamental principles behind each model, the methodology for coupling them, and the iteration scheme employed to ensure convergence. Section III presents and analyzes the results obtained from the coupled calculations, focusing on how CRUD deposition affects axial and radial power distributions, alters local fuel-rod dimensions, and induces neighboring effects. Additionally, it examines the feedback between the power and temperature distributions of the assembly and their influence on CRUD growth at both global and local scales. These findings are discussed to highlight key insights and their broader implications. Finally, Sec. IV summarizes the major conclusions, critically reviews the limitations of the study and provides recommendations for future research to further refine and expand the framework.

II. METHODS

This framework utilizes an internally coupled computational approach, in which the neutronic field (power distribution), the temperature field, and the CRUD deposition field are simultaneously updated in memory and iteratively solved using a Picard-based coupling scheme. To overcome the multiscale-modeling challenges associated with CRUD deposition, the framework implements a background-mesh technique, which applies identical mesh resolution to regions with spatially nonuniform CRUD growth patterns, unifying geometric variations across different regions and reducing computation time while introducing only minimal deviations.

A. Neutronics simulations

The neutronics (N) model employed in the coupling simulation, VITAS, is a three-dimensional (3D) deterministic neutron-transport simulation code developed by Shanghai Jiao Tong University, based on the heterogeneous variational nodal method (HVNM) [37]. VITAS is developed based on the second-order neutron-transport equation (NTE) under the assumption of isotropic scattering. The

multigroup second-order NTE is articulated as follows:

$$-\mathbf{\Omega} \cdot \nabla [\Sigma_t^{-1}(\mathbf{r})\mathbf{\Omega} \cdot \nabla \psi^+(\mathbf{r}, \mathbf{\Omega})] + \Sigma_t(\mathbf{r})\psi^+(\mathbf{r}, \mathbf{\Omega}) = \int_{\mathbf{\Omega}'} \Sigma_s(\mathbf{r}, \mathbf{\Omega}' \rightarrow \mathbf{\Omega}) \psi^+(\mathbf{r}, \mathbf{\Omega}') d\mathbf{\Omega}' + Q^+(\mathbf{r}, \mathbf{\Omega}), \quad (1)$$

$$\psi^-(\mathbf{r}, \mathbf{\Omega}) = -\Sigma_t^{-1}(\mathbf{r})\mathbf{\Omega} \cdot \nabla \psi^+(\mathbf{r}, \mathbf{\Omega}), \quad (2)$$

where $\psi^+(\mathbf{r}, \mathbf{\Omega})$ represents the even-parity neutron angular flux, $\psi^-(\mathbf{r}, \mathbf{\Omega})$ denotes the odd-parity neutron angular flux, $\mathbf{r}$ is the spatial location, $\mathbf{\Omega}$ is the neutron travel direction, $\Sigma_t(\mathbf{r})$ and $\Sigma_s(\mathbf{r})$ are the macroscopic total and isotropic scattering cross sections, and $S(\mathbf{r})$ is the group source, consisting of fission and outer sources.

The neutron-transport code achieves 3D neutron-flux solutions by reformulating the governing equations into a series of corresponding matrix systems:

$$j^+ = \mathbf{B}q + \mathbf{R}j^-, \quad (3)$$

$$\phi = \mathbf{V}q - \mathbf{C}(j^+ - j^-), \quad (4)$$

where j^+ and j^- denote the vectors of the expansion moments of outgoing and incoming partial currents along the nodal surfaces, respectively, and $\mathbf{B}$, $\mathbf{R}$, $\mathbf{V}$, and $\mathbf{C}$ are nodal-response matrices, which are coefficient matrices solely related to the nodal geometry and macroscopic cross sections (XSs).

B. Thermal-hydraulics simulations

The thermal-hydraulics (TH) model employs a multichannel approach [38] to compute coolant-temperature distributions and channel pressure drops. For each coolant channel, the solution is obtained by simultaneously solving the mass-conservation, energy-conservation, and momentum-conservation equations. To model heat conduction in the fuel, the framework implements the half-boundary method (HBM) [39]. This approach introduces an auxiliary variable that transforms the governing heat-transfer equation into a system of first-order partial differential equations. This transformation not only simplifies the mathematical representation of the problem but also significantly reduces the dimensionality of the coefficient matrix, thereby enhancing computational efficiency.

1. Multichannel model

The coolant mass, energy, and momentum conservation relations are given by

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial z}(\rho u) = 0, \quad (5)$$

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial z}(\rho u h) = Q_{\text{cool}}, \quad (6)$$

and

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial z}(\rho u^2) + \frac{\partial P_{\text{fric}}}{\partial z} + g\rho + \frac{\partial P}{\partial z} = 0, \quad (7)$$

where ρ represents the coolant density, u represents the coolant flow rate, h represents the coolant enthalpy, P_{fric} represents the frictional pressure drop, and P represents the pressure.

2. Heat-conduction model

To solve the fuel-temperature distribution, the HBM is applied to solve the heat-conduction equation. The heat-conduction equation in cylindrical coordinates can be written as

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \kappa_f \frac{\partial T}{\partial r} \right) + q''(r) = 0, \quad (8)$$

where κ_f is the thermal conductivity and $q''(r)$ is the volumetric heat-generation rate of the fuel rod.

This method introduces variable V into the governing heat-transfer equation (the variable V is the heat flux),

$$V = \kappa_f(T, r) \frac{\partial T}{\partial r}, \quad (9)$$

transforming Eq. (8) into a system of first-order partial differential equations.

By applying finite differences to the differential equations and integrating over the radial coordinate, each mesh has

$$\begin{cases} 2r_{i+1}V_{i+1} = 2r_iV_i + (r_i^2 - r_{i+1}^2)q''(r_i), \\ T_{i+1} - \frac{1}{2} \frac{\Delta r}{\kappa_{i+1}} V_{i+1} = T_i + \frac{1}{2} \frac{\Delta r}{\kappa_i} V_i. \end{cases} \quad (10)$$

By substituting the boundary conditions into Eq. (12), the temperature and heat flux at one side can be determined. The final equation can be obtained as

$$\begin{cases} T_i = c_{1i}T_0 + c_{2i}V_0 + d_{1i}, \\ V_{i+1} = c_{3i}T_0 + c_{4i}V_0 + d_{2i}, \end{cases} \quad (14)$$

where

$$\begin{aligned} c_{1i} &= 1, \quad c_{2i} = \sum_{n=1}^i \left[\left(\frac{1}{2} \frac{r_n \Delta r_n}{r_{n+1} \kappa_{n+1}} + \frac{1}{2} \frac{\Delta r_n}{\kappa_n} \right) \frac{r_1}{r_n} \right], \quad c_{3i} = 0, \quad c_{4i} = \frac{r_1}{r_i}, \\ d_{1i} &= \sum_{m=1}^{i-1} \left\{ -\frac{r_m^2(r_{m+1} + r_m)}{4r_{m+1}\kappa_m} q''(r_m) - \frac{r_{m+1} + r_m}{4r_{m+1}} q''(r_m) \Delta r_m \sum_{n=m}^{i-1} \left[\left(\frac{r_n \Delta r_n}{r_{n+1} \kappa_n} + \frac{\Delta r_n}{\kappa_n} \right) \frac{r_1}{r_n} \right] \right\}, \\ d_{2i} &= \sum_{n=1}^{i-1} -\frac{r_{n+1} + r_n}{r_{n+1}} q''(r_n) \Delta r_n. \end{aligned}$$

Organizing them into matrix form,

$$\begin{bmatrix} 0 & 2r_{i+1} \\ 1 & -\frac{1}{2} \frac{\Delta r}{\kappa_{i+1}} \end{bmatrix} \begin{bmatrix} T_{i+1} \\ V_{i+1} \end{bmatrix} = \begin{bmatrix} 0 & 2r_i \\ 1 & \frac{1}{2} \frac{\Delta r}{\kappa_i} \end{bmatrix} \begin{bmatrix} T_i \\ V_i \end{bmatrix} + \begin{bmatrix} (r_i^2 - r_{i+1}^2) q''(r_i) \\ 0 \end{bmatrix}. \quad (11)$$

Setting

$$A = \begin{bmatrix} 0 & 2r_{i+1} \\ 1 & -\frac{1}{2} \frac{\Delta r}{\kappa_{i+1}} \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 2r_i \\ 1 & \frac{1}{2} \frac{\Delta r}{\kappa_i} \end{bmatrix}, \\ C = \begin{bmatrix} (r_i^2 - r_{i+1}^2) q''(r_i) \\ 0 \end{bmatrix},$$

the recurrence relation can be derived as follows:

$$\begin{bmatrix} T_{i+1} \\ V_{i+1} \end{bmatrix} = A_i^{-1} B_i \begin{bmatrix} T_i \\ V_i \end{bmatrix} + A_i^{-1} C_i. \quad (12)$$

Under given boundary conditions, the temperature and heat-flux density at each node in the heat-conduction equation can be calculated through iterative computations of Eq. (12). For a certain fuel rod, there is $V_1 = 0$ at the center; based on the heat-transfer relationship between the surface cladding and the coolant, it could be derived as

$$-V_n = h(T_n - T_{\text{cool}}), \quad (13)$$

where T_{cool} is the coolant temperature and h is the heat-transfer coefficient between the cladding and the coolant.

3. Subcooled nucleate boiling

As previously mentioned in Fig. 1(a), SNB plays a critical role in the CRUD deposition process, and whether SNB occurs in each mesh is a key factor in the CRUD growth model calculations. During the coupling process, the Jens-Lottes boiling heat-transfer correlation [40] is introduced to determine whether the cladding surface temperature has reached the onset of SNB. The Jens-Lottes correlation is given as follows:

$$\Delta T_{\text{sat}} = t_w - t_s = 25 \left(\frac{q}{10^6} \right)^{0.25} \exp \left(\frac{-p}{6.2} \right), \quad (15)$$

where ΔT_{sat} is the wall superheat (K), t_w is the temperature of the cladding surface, t_s is the temperature of the coolant, q is the heat flux (W/m^2), and p is the pressure (MPa).

C. CRUD simulations

The CRUD model incorporates both a CRUD growth model and a CRUD-concentration model to evaluate the concentration of species within the CRUD deposition layer. The growth model tracks the CRUD thickness evolution through two primary mechanisms: chemical precipitation and particulate accumulation. Concurrently, the concentration model employs an enhanced Cohen-Pan framework [26,41] to solve the coupled thermal-hydraulics balance equations and chemical-equilibrium conditions surrounding the CRUD chimney structures.

1. CRUD growth model

In PWRs, corrosion products derived from the primary coolant circuit are transported into the reactor core and subsequently deposited onto fuel-rod surfaces via two dominant mechanisms: (1) chemical precipitation of dissolved species and (2) particulate deposition driven by Brownian motion. Under the SNB condition, the deposition process is substantially intensified due to localized solute concentration effects and an enhanced coupled turbulence-microconvection effect at the fuel cladding surface.

The soluble-products deposition rate at a quasisteady state is expressed as [42,43]

$$m_s = \sum_i [(h_{mt,s} c_{p,f,i} - h_{mt,s} c_{p,w,i} + h_{B,s} c_{p,w,i}) M_i], \quad (16)$$

where m_s is the soluble corrosion-product deposition rate, M is the molecular weight of species, $h_{mt,s}$ is the soluble-products mass-transfer coefficient, $h_{B,s}$ is the subcooled-boiling mass-transfer coefficient, i represents the soluble corrosion-product species, $c_{p,f,i}$ is the coolant soluble-species concentration, and $c_{p,w,i}$ is the surface soluble-species concentration.

For regions with varying boiling conditions, the transfer coefficient is calculated as

$$h_{mt,s} = 0.5f v \left(\frac{\mu_i}{\rho_i D_i} \right)^{-\frac{2}{3}}, \quad (17)$$

$$f = (1.58 \lg(\text{Re}) - 3.28)^{-2}, \quad (18)$$

where D is the species diffusion coefficient, f is the fanning friction factor, v is the flow velocity, μ is the species dynamic viscosity, ρ is the density; and Re is the Reynolds number. For regions where SNB occurs, the mass transfer induced by boiling effects is taken into account:

$$h_{B,s} = \frac{q}{\rho_i h} h_{mt,s}, \quad (19)$$

where q is the evaporative heat flux and h is the latent heat of vaporization.

The deposition rate per unit area of particle corrosion products is computed as [42]

$$m_p = (h_{mt,p} c_{p,w} + h_{B,p} c_{p,w}) m, \quad (20)$$

$$h_{mt,p} = 0.5f v \left(\frac{\mu}{\rho D_p} \right)^{-\frac{2}{3}}, \quad (21)$$

where m_p is the deposition rate per unit area of particle corrosion products, $c_{p,w}$ is the surface particle concentration, $h_{mt,p}$ is the particle mass-transfer coefficient, $h_{B,p}$ is the subcooled-boiling mass-transfer coefficient, and D_p is the particle diffusion coefficient.

The transport of particulate material to the cladding surface driven by turbulence is identical to that of soluble material, with the exception that the diffusion constant employed to determine the mass-transfer rates is derived from the Stokes-Einstein relationship:

$$D_p = \frac{k_b T_f}{6\pi \mu_f r_p}, \quad (22)$$

where k_b is the Boltzmann constant, r_p is the particle radius, μ_f is the coolant dynamic viscosity, and T_f is the cladding surface coolant temperature. Eventually, the CRUD mass growth equation is formulated as the summation of the deposition of particulate corrosion products and soluble corrosion products:

$$\dot{m} = m_s + m_p, \quad (23)$$

where m_p the deposition rate per unit area of particulate corrosion products and m_s is the deposition rate per unit area of soluble corrosion products.

2. CRUD-concentration model

The CRUD-concentration model first solves for the temperature distribution within the CRUD layer. Subsequently, convection-diffusion equations and chemical-equilibrium equations are solved based on the computed

temperature field to determine the internal concentration profiles of the chemical species. The temperature distribution is derived using a generalized Cohen-type and Pan-type model [22], in which the system is assumed to be in a quasisteady state. This is achieved by solving the heat-conduction equation, with the thermal conductivity of CRUD calculated as follows:

$$\nabla \cdot (\kappa_{\text{CRUD}} \nabla T) + q'' = 0, \quad (24)$$

$$\kappa_{\text{CRUD}} = \frac{(2 - D_f) \varepsilon \lambda_{\text{max}}^{D_T-1} \left[1 - \left(\frac{\lambda_{\text{min}}}{\lambda_{\text{max}}} \right)^{D_T-D_f+1} \right]}{L_{\text{CRUD}}^{D_T-1} (D_T - D_f + 1) \left[1 - \left(\frac{\lambda_{\text{min}}}{\lambda_{\text{max}}} \right)^{2-D_f} \right]} \kappa_f + (1 - \varepsilon) \kappa_s, \quad (25)$$

where κ_{CRUD} is the thermal conductivity of CRUD, κ_f and κ_s are the thermal conductivity of the CRUD coolant and the metal solid skeleton, λ_{max} and λ_{min} are the maximum and minimum pore diameter, D_f and D_T are the fractal dimension and the tortuosity dimension, and L is the path length of the coolant. A detailed derivation can be found in fractal theory [24].

In the model, the chemical-reaction equilibria are primarily governed by temperature. To approximate the equilibrium constants of these reactions, the model employs a trinomial correlation [44]:

$$\log K_i = C_1 + \frac{C_2}{T} + C_3 \log T. \quad (26)$$

The chemical equilibrium of various reactions in the coolant is solved to determine the state of the coolant solutes, which subsequently enables the calculation of concentrations for both soluble and insoluble particulate species in the governing equations. The module accounts for multiple chemical interactions, including reactions between water and ionic species (such as water ionization, iron-water interactions, nickel-water interactions, and boric acid reactions) as well as precipitation reactions that form insoluble corrosion products. A comprehensive list of all considered reactions is provided in Appendix B. Due to the tortuous microstructure within porous CRUD depositions, the diffusion coefficient must be corrected as described in Eq. (27). Furthermore, internal boiling leads to solute concentrations that exceed those in the bulk coolant by several orders of magnitude. This elevated solute concentration increases the saturation temperature of the coolant, which in turn influences internal boiling behavior. Therefore, the effect of solute concentration on saturation temperature must be accounted for. Based on the balance of water and steam, the relationship between saturation temperature and solute concentration is derived from the chemical potential, as expressed in Eq. (28). By solving this thermodynamic equation, the correlation between

the solute concentration and the saturation temperature at 15.5 MPa is determined:

$$D_i = D_w \frac{\varepsilon}{\tau}, \quad (27)$$

$$\mu_{c,w}(P_0) + RT_{\text{sat}} \ln \frac{m_w}{m_w + \sum m_{\text{solute}}} \bigg|_P = \mu_{c,v}(P), \quad (28)$$

where D_w is the diffusion coefficient in bulk coolant, ε is the CRUD permeability, τ is the tortuosity factor, $\mu_{c,w}$ and $\mu_{c,v}$ are the chemical potential of water and steam, and m_w and m_{solute} are the mass concentrations of water and solute.

With all equations considered, the model solves the solute concentration (29) in a quasisteady state:

$$\frac{\partial c_i}{\partial t} = [(\vec{u} \cdot \vec{n}) - \nabla D_i] \nabla c_i + \sum_i (c_i - c_{i,\text{sink}}), \quad (29)$$

where D_i presents the diffusion loss of concentration and $c_{i,\text{sink}}$ is the mass-concentration sink due to chemical reaction.

To simulate boron transport within the CRUD layer, a one-dimensional virtual mesh is implemented with a radial resolution of 0.8 μm per cell. This resolution maintains temperature-prediction errors within 1% compared to experimental data [35] across typical CRUD thickness ranges (20–200 μm), with constrained memory allocation (e.g., reducing to 0.4 μm would increase memory requirements by 200% for negligible improvement in accuracy.)

D. Background-mesh method

In neutronics-CRUD coupling, the primary feedback mechanism stems from boron-hideout effects on power distribution. The CRUD model resolves boron concentration at the micrometer (μm) scale but this fine resolution introduces significant discrepancies when applied to fuel rods and assemblies modeled at the centimeter (cm) scale. In the neutronics model, such fine-grained resolution reduces computational efficiency and increases the risk of numerical instability. To mitigate this issue, a background-mesh layer is introduced to homogenize the boron-concentration distribution between the CRUD and surrounding coolant.

For a given reaction type α , the cross sections in the background layer are calculated using the following equation:

$$\Sigma_{\alpha,bg} = \frac{\int_{D_{\text{CRUD}}} \int_{\Delta E_g} N_{\text{CRUD}}(r, E) \sigma_{\alpha,\text{CRUD}}(E) \phi(r, E) dE dr}{\int_{D_{\text{CRUD}}+D_{\text{cool}}} \int_{\Delta E_g} \phi(r, E) dE dr} + \frac{\int_{D_{\text{cool}}} \int_{\Delta E_g} N_{\text{cool}}(E) \sigma_{\alpha,\text{cool}}(E) \phi(r, E) dE dr}{\int_{D_{\text{CRUD}}+D_{\text{cool}}} \int_{\Delta E_g} \phi(r, E) dE dr}, \quad (30)$$

where the $\Sigma_{\alpha,bg}$ are the macroscopic cross sections for the background layer.

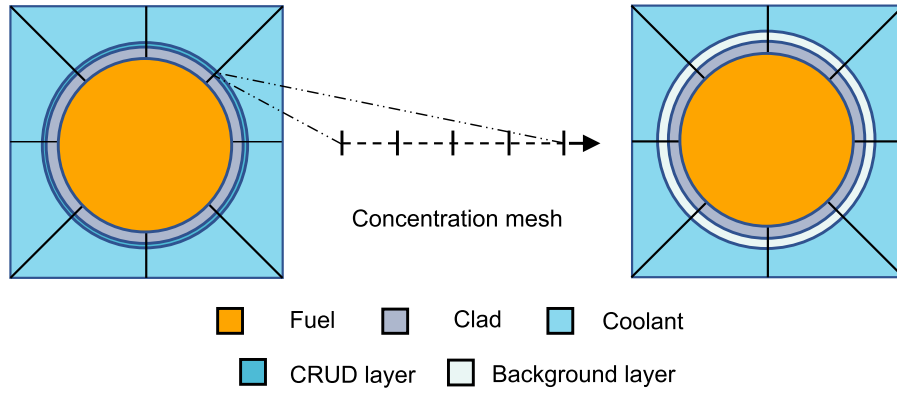


FIG. 2. The virtual concentration mesh describes the detailed boron-concentration gradients and is homogenized with part of the coolant in the background layer.

This method effectively preserves critical boron-concentration data while mitigating issues caused by excessive grid-size disparities. Benchmark studies on PWR fuel-rod pin cells have confirmed that the 500- μm background mesh delivers optimal performance [10.2% faster computation, 68 percent mille (pcm) eigenvalue error] and it has been adopted for all simulations. In the study, a 500- μm background mesh is employed and it reduces computational time by over 10%, with eigenvalue errors remaining below 60 pcm. The background layer is illustrated in Fig. 2. The dimensional changes caused by CRUD deposition also present challenges for heat-transfer modeling. At the microscale level, the temperature distribution within the CRUD layer is governed by the CRUD-concentration model, which uses boundary conditions from the thermal-hydraulics model to conduct heat-transfer calculations. At the macroscale level, considering the small dimensions and relatively minor impact of CRUD, a modified convective heat-transfer coefficient between the coolant and fuel cladding surface is implemented to represent the thermal effects of CRUD, as demonstrated in the previous research [29].

E. Coupling methodology

In the NTE, for a certain type of reaction α , the cross sections are considered as

$$\Sigma_{\alpha} = \frac{\int_D \int_{\Delta E_g} N(r, E) \sigma_{\alpha}(E, T) \phi(r, E) dE dr}{\int_D \int_{\Delta E_g} \phi(r, E) dE dr} \equiv \Sigma_{\alpha}(N, T), \quad (31)$$

where $\sigma_{\alpha}(E, T)$ denotes the microscopic cross section for reaction type α , N represents the material nuclide density, and T represents the material temperature. For the current simulations, all microscopic cross-section data have been extracted from the ENDF/B-VII.1 nuclear data library and

processed by the NJOY software package [45]. The steady-state NTE can be written in operator form as

$$\mathcal{N}(N, T)\phi = \lambda \mathcal{F}_v(N, T)\phi, \quad (32)$$

where $\mathcal{N}$ represents the nonfission transport terms, $\mathcal{F}_v$ represents fission neutron production terms, ϕ is the neutron flux, and λ is the eigenvalue reciprocal.

The fission power needs to be associated with the heat emission, which is represented as

$$q'' = \mathcal{F}_k(N, T)\phi, \quad (33)$$

where q'' represent local heat emission and $\mathcal{F}_k$ represents fission heat production terms.

In the thermal-hydraulics simulation and the CRUD internal-heat simulation, the steady-state heat-diffusion equation is written in operator form as

$$\mathcal{L}(T)T + q'' = 0, \quad (34)$$

where $\mathcal{L}$ is the diffusion operator.

The CRUD chemical reaction equilibrium is written in operator form as

$$\mathcal{C}_{\text{sink}}(T, N) + \mathcal{L}(N) = 0. \quad (35)$$

The multiphysics analysis system can be described in the equation as

$$\begin{pmatrix} \phi \\ \lambda \\ T \\ N \end{pmatrix} = F \begin{pmatrix} \mathcal{N}(N, T)\phi - \lambda \mathcal{F}_v(N, T)\phi \\ \mathcal{L}(T)T - \mathcal{F}_k(N, T)\phi \\ \mathcal{C}_{\text{sink}}(T, N) + \mathcal{L}(N) \end{pmatrix}. \quad (36)$$

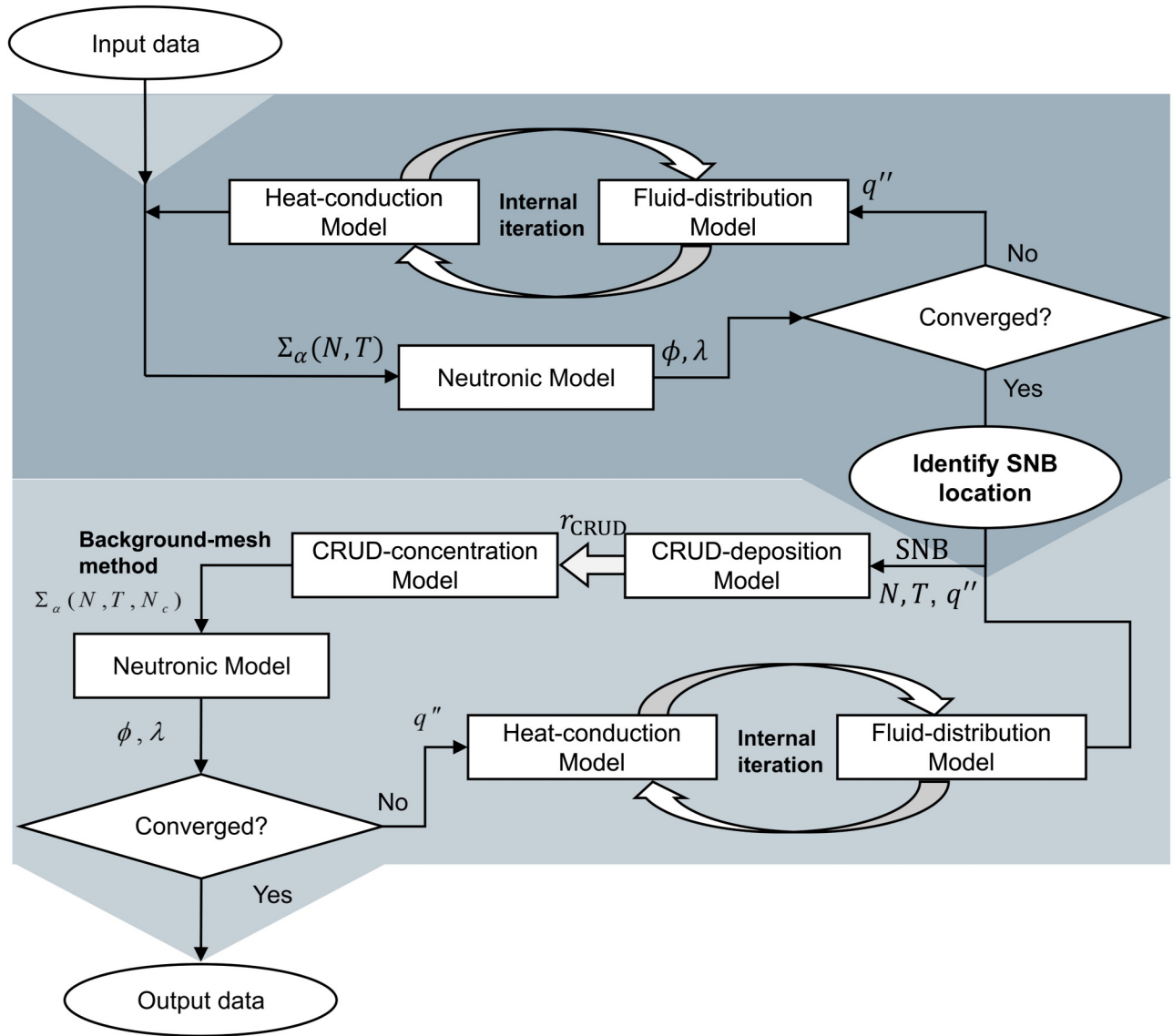


FIG. 3. The coupling scheme employs a fixed SNB location to circumvent convergence difficulties.

The system uses Picard iteration to solve the equation. In each step, the iteration ideology can be described as

$$\begin{pmatrix} \phi^{(n)} \\ \lambda^{(n)} \\ T^{(n)} \\ N^{(n)} \end{pmatrix} = F \begin{pmatrix} \mathcal{N}(N^{(n-1)}, T^{(n-1)})\phi - \lambda \mathcal{F}_v(N^{(n-1)}, T^{(n-1)})\phi \\ \mathcal{L}(T)T - \mathcal{F}_\kappa(N^{(n-1)}, T^{(n-1)})\phi^{(n)} \\ \mathcal{C}_{\text{sink}}(T^{(n)}, N^{(n-1)}) + \mathcal{L}(N^{(n-1)}) \end{pmatrix}. \quad (37)$$

The work flow of the coupled simulation is illustrated in Fig. 3. Initially, a Picard iteration scheme is applied between the neutronics model and the thermal-hydraulics

model. In each iteration step, both models are solved independently to convergence before exchanging temperature, density, and power-distribution data. This iterative process continues until the eigenvalues and neutron flux converge, yielding a baseline solution without CRUD effects for comparison. This solution, comprising the approximate SNB conditions, the temperature field, and the physical field distribution, serves as the initial condition for the subsequent neutronics-TH-CRUD coupled calculation, significantly reducing the required iterations. Next, the identified CRUD deposition locations and corresponding thermal-hydraulics parameters are input into the CRUD-deposition model, which computes the CRUD layer thickness, while the CRUD-concentration model evaluates the nuclide density distribution within the CRUD region. The background-mesh method is then used to generate cross

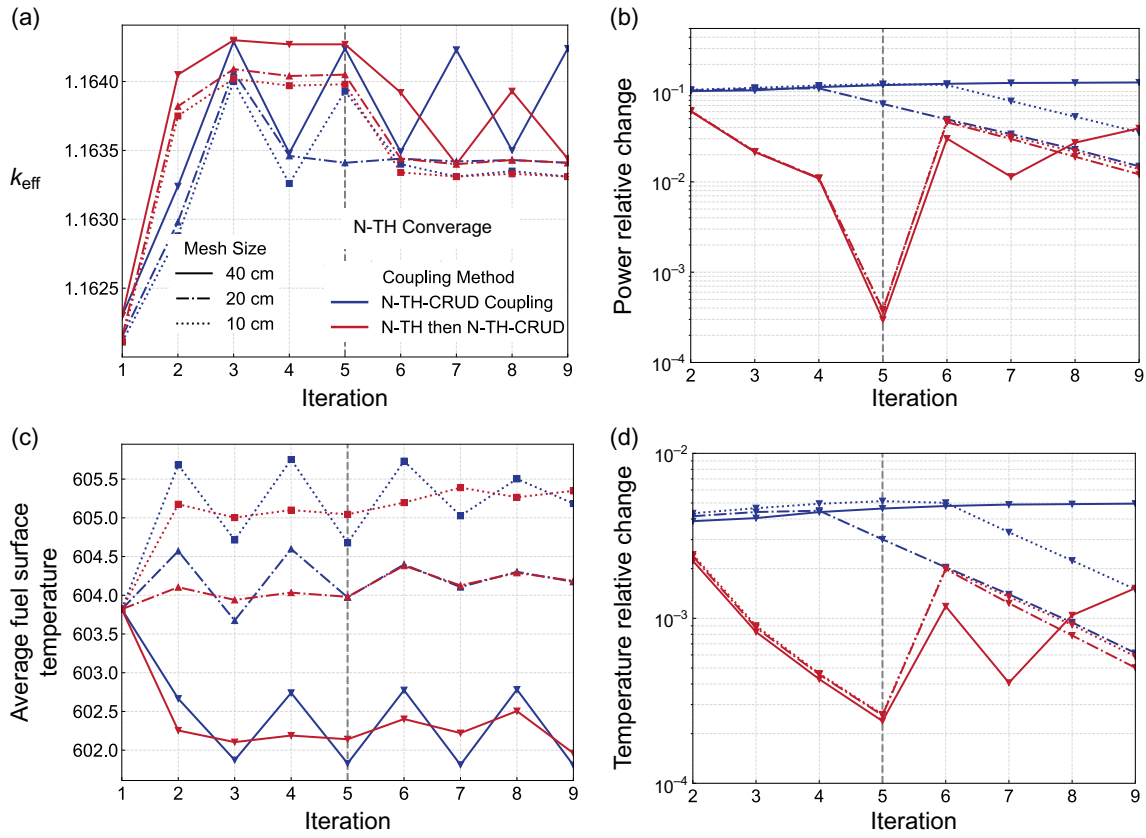


FIG. 4. Coupling numerical stability and sensitivity to mesh size. (a) The convergence of k_{eff} . (b) The power-convergence trend. (c) The convergence of the fuel surface temperature. (d) The fuel surface temperature convergence trend.

sections for the CRUD-affected regions, which are passed to the neutron-transport calculations. The neutronics and thermal-hydraulics models are reexecuted to update the physical fields iteratively. This cycle repeats until full convergence is achieved.

To assess the robustness of the Picard iteration scheme, analyses of numerical stability, mesh sensitivity, and computational efficiency have been performed for single-fuel-rod simulations. For coupled simulations, axial temperature distributions exhibit significantly larger variations compared to radial directions due to geometric symmetry. Radially, temperature field meshes assigned to individual fuel rods and associated coolant regions provide sufficient resolution. Consequently, focused sensitivity analyses have been conducted exclusively on axial discretization where greater gradients necessitate rigorous assessment.

As depicted in the figure, the convergence behavior shows a significant dependence on axial discretization. With 40-cm axial meshes [Fig. 4(a)], k_{eff} evolution during full N-TH-CRUD coupling exhibits oscillations reaching 50 pcm, preventing convergence. Finer 10-cm and 20-cm meshes maintain k_{eff} variations within 5 pcm, indicating sufficient spatial resolution for stable coupling. To evaluate the convergence trend of the physics field, the relative

change is expressed as

$$\text{relative change} = \frac{\|\phi^{(n)} - \phi^{(n-1)}\|}{\|\phi^{(n-1)}\|}, \quad (38)$$

where $\|\cdot\|$ denotes the Frobenius norm and $\phi^{(n)}$ is the result of the physics field in iteration step n .

Power-distribution analysis [Fig. 4(b)] reveals the convergence trend of the neutronic field. N-TH-only coupling achieves marginal convergence at 40-cm resolution, while both the sequential N-TH $\rightarrow$ N-TH-CRUD and direct N-TH-CRUD strategies diverge, with the relative change exceeding 10%. For the fuel surface temperatures [Fig. 4(c)], differences between 10-cm and 20-cm resolutions remain below 1 K. Convergence-rate comparisons [Fig. 4(d)] show that the 10-cm mesh converges more slowly than the 20-cm discretization due to higher resolution, with both sequential and direct coupling strategies exhibiting this trend. In Figs. 4(b) and 4(d), we indicate that the sequential (N-TH $\rightarrow$ N-TH-CRUD) and direct N-TH-CRUD strategies have similar convergence efficiencies, with the sequential approach additionally providing converged N-TH reference solutions. The computational time for the single-fuel-rod simulation benchmark is given

TABLE I. Benchmark calculation time.

Mesh size	Strategy	Time (core-hour)	Strategy	Time (core-hour)
10 cm	Sequential	296.05	Direct	327.21
20 cm	Sequential	82.93	Direct	88.31
40 cm	Sequential	57.22	Direct	63.72

in Table I. Considering the trade-off between computational efficiency and accuracy, the 20-cm axial mesh discretization has been selected for the coupled analysis as the optimal choice.

III. RESULTS AND DISCUSSION

In this study, the CRUD deposition rate is represented as an equivalent thickness accumulated over 180 days of steady-state operation. The quasi-steady-state corrosion-deposition process is approximated as a steady-state process to simplify the computational approach, while the boron distribution derived from the operating conditions is integrated into the analysis. The CRUD growth patterns under these coupled physical fields have been systematically analyzed. Detailed investigations have been conducted on individual fuel rods within the assembly to identify CRUD growth mechanisms and characteristics specific to PWR operating conditions. The design parameters of the fuel assembly have been partially derived from the virtual environment for reactor applications (VERA) benchmark problem [46], which is shown in Table II. Modeling details of the assembly geometry are provided in Appendix A.

TABLE II. Assembly design parameters: ppm, parts per million.

Parameter	Value
Fuel radius	0.4096 cm
Cladding radius	0.475 cm
Background-mesh radius	0.525 cm
Fuel material	UO ₂
Fuel enrichment	3.1%
Cladding material	Zircaloy-4
Assembly height	380 cm
Coolant inlet temperature	565 K
Inlet mass flow rate	24.056 kg/s
Pressure	15.5 MPa
Assembly power	19.31 MW
Soluble boron concentration	1300 ppm
Steady operation time	180 days
Axial discretization	20 meshes

TABLE III. Comparison of CRUD-related parameters.

Parameter	N-TH	N-TH-CRUD
Axial offset (AO)	−2.28%	−6.29%
k_{eff}	1.16184	1.15891
Power peak	189 cm	169 cm
Normalized peak power	1.409	1.412
Power of the highest-power rod	70.565 kW	70.578 kW
Power of the lowest-power rod	61.732 kW	61.748 kW
Average coolant temperature	587.56 K	587.97 K
Maximum surface heat flux	914.51 kW/m ²	916.13 kW/m ²

A. Coupling results

The CRUD-coupled neutronics-thermal simulation achieved convergence within four Picard iterations, satisfying the eigenvalue convergence criterion of 1×10^{-4} with a final eigenvalue k_{eff} of 1.15891. For reference, a baseline simulation without CRUD effects yielded a converged eigenvalue of 1.16184, indicating a 293-pcm reactivity reduction attributable to the CRUD effects. The 293-pcm reactivity shift from CRUD deposition is operationally acceptable, being below the typical 500-pcm limit for monthly surveillance [27]. For reactor operation, such reactivity variations can be compensated through standard control mechanisms, including chemical shim control and control rod control. Table III presents a comparison of key results related to CRUD, while Fig. 5 illustrates the power-distribution analysis under CRUD-affected conditions.

The 3D normalized power distribution with the CRUD effect is depicted in Fig. 5(a): the normalized power density is the ratio of the local power density to the average assembly power density while the dark blue regions denote guide-tube locations, which remain non-power-producing during reactor operation. These structural components play a crucial role in core power-distribution management through control-rod operation and burnable poison placement. In Fig. 5(b), we display the axial normalized power distribution under three-field coupling conditions (N-TH-CRUD chemistry), showing a downward shift from the theoretical cosine distribution that serves as the baseline for an ideal reactor core without CRUD effects. The power peak occurs at 169-cm elevation in the fuel assembly. For quantitative evaluation of the axial power-distribution deviations, we have employed the axial offset (AO) parameter following Westinghouse's established methodology:

$$\text{AO} = \frac{(P_t - P_b)}{(P_t + P_b)} \times 100\%, \quad (39)$$

where P_t is the integrated power of the top half and P_b is the integrated power of the bottom half.

The fuel assembly exhibits an AO of −6.29%, compared to −2.28% under Doppler feedback alone (without CRUD effects). Experimental data from the Electric Power

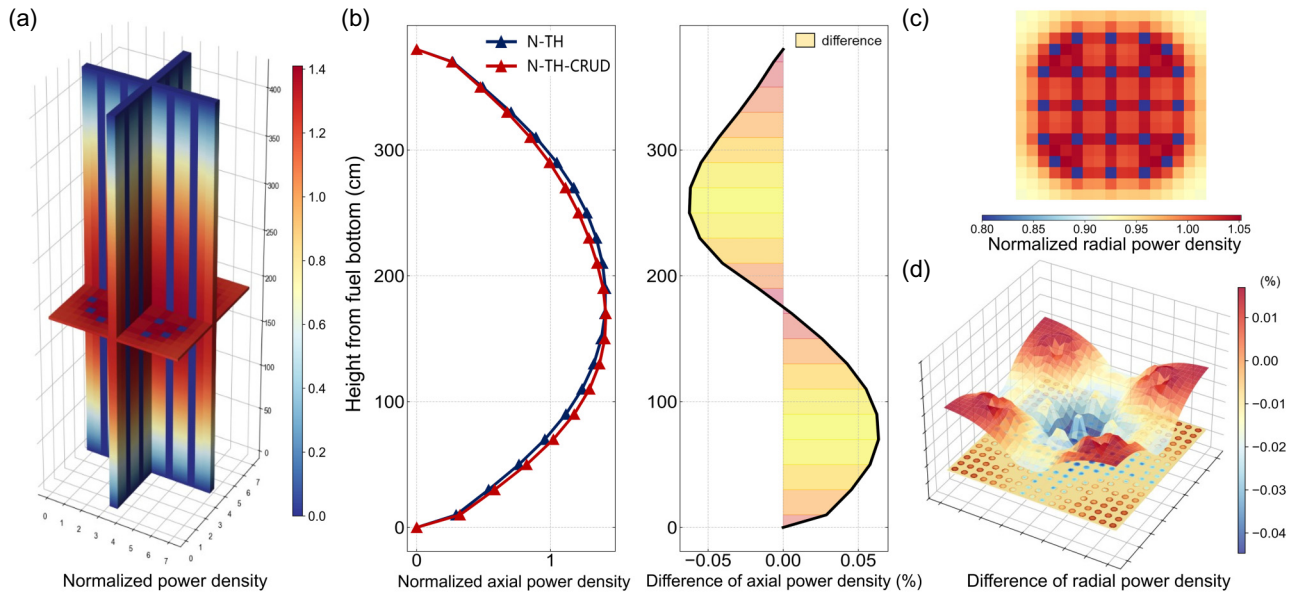


FIG. 5. Coupling simulation results and comparative analysis. (a) The three-dimensional (3D) power distribution under the influence of CRUD. (b) The axial normalized power density: baseline case [neutronics–thermal–hydraulics (N-TH) coupling] versus the CRUD case [neutronics–thermal hydraulics–CRUD (N-TH-CRUD) coupling]. (c) The axially integrated radial power distribution. (d) The radial power discrepancy induced by CRUD effects: baseline case versus CRUD case.

Research Institute (EPRI) [27] demonstrate that a core-average boron deposition of 2267.96 mg per fuel assembly induces an AO of approximately 5%. In the present simulation, the total boron deposition of 2574.43 mg exhibits an AO shift of -6.29% , which aligns with the expected trend. CRUD deposition leads to power suppression in the (250–300)-cm axial region. This phenomenon also results in a downward shift of the power peak location from 189 to 169 cm, coupled with an increase in the relative power peak from 1.409 to 1.412. In Fig. 5(c), we illustrate the axially integrated radial power distribution of the fuel assembly, primarily governed by its geometric configuration. The assembly incorporates 25 guide tubes, arranged in two distinct patterns—an outer arc-shaped distribution and an inner rectangular configuration. Beyond the outer arc-shaped guide-tube region, the fuel-rod power gradually decreases with radial distance from the geometric center. Within the inner rectangular region, fuel rods directly adjacent to guide tubes exhibit higher power levels (3% greater) compared to diagonally adjacent rods due to enhanced thermal-neutron flux near moderator-filled guide tubes. Notably, the arc-shaped guide-tube regions at each assembly corner contain zones with both direct and diagonal adjacency to guide tubes, producing localized power peaks with relative values of approximately 1.052. Conversely, the four corner regions of the assembly demonstrate relative power minima around 0.9203. These spatial variations arise from neutron moderation effects: water in the guide tubes provides a high neutron-scattering cross section (Σ_s), increasing the thermal-neutron population

in adjacent fuel rods. The resulting flux elevation, combined with the larger fission cross section (Σ_f) of thermal neutrons, drives higher fission rates and power generation in guide-tube-proximate regions. This phenomenon is characteristic of PWR fuel designs, where the moderator distribution directly influences the localized power shaping. In Fig. 5(d), we present the variations of the axially integrated power distribution across the full fuel assembly between the CRUD-affected and CRUD-free scenarios. In Fig. 5(d), we demonstrate the localized radial power deviations, which range from $+11$ W to -25 W, revealing a distinct pattern of power depression in central fuel rods accompanied by power elevation in peripheral regions. When normalized against the total assembly power of 19.31 MW, these deviations correspond to relative variations of approximately $+0.06\%$ to -0.14% , with an overall impact magnitude of just 0.04% . This minimal variation confirms that CRUD-induced power-redistribution effects remain well within acceptable operational margins for this fuel-assembly design.

The CRUD-induced N-TH coupling simulations provide insights for analyzing the thermal-hydraulics behavior of the assembly. In Fig. 6, we present a comparative analysis of the axial profiles for key thermodynamic parameters derived from radial integration. The fuel-rod surface-temperature distribution in Fig. 6(a) reflects the combined effects of internal-fission heat generation, thermal conduction through the fuel, and convective and/or boiling heat transfer to the coolant, reaching its peak of 618.2 K at 273 cm elevation. CRUD deposition induces

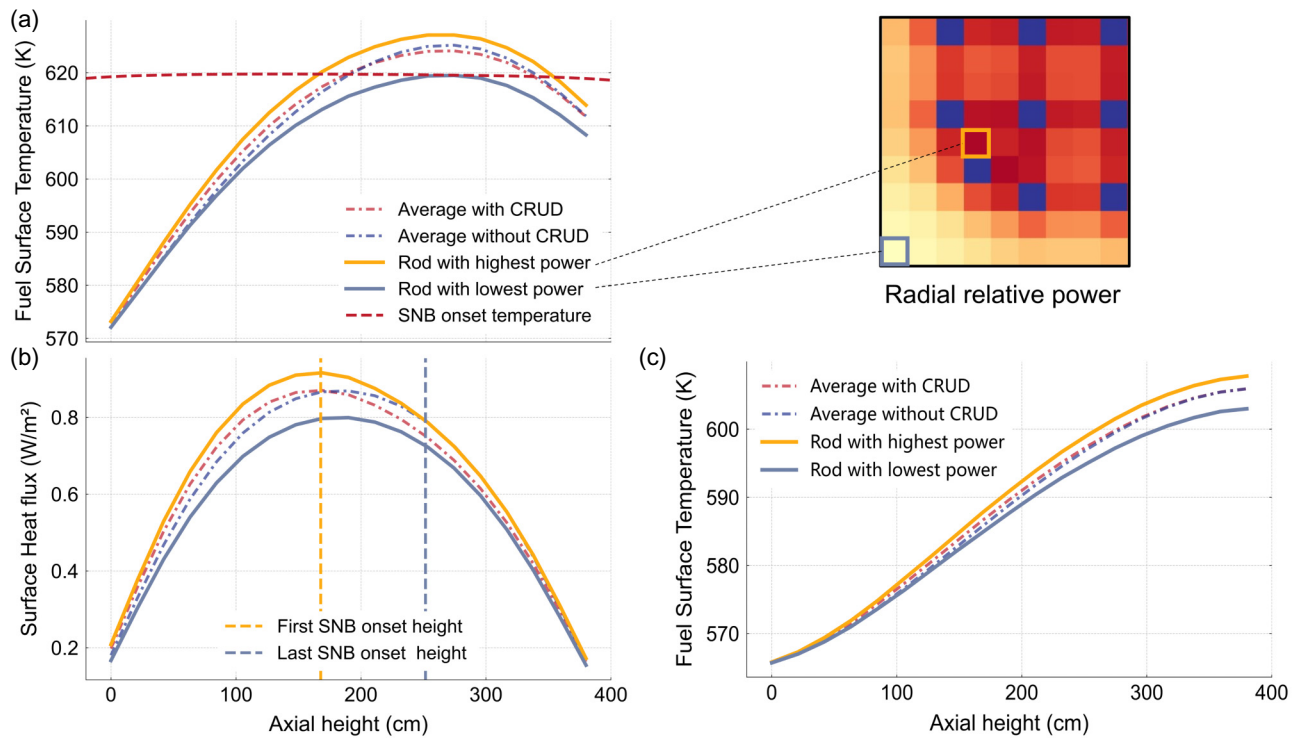


FIG. 6. A comparison of the thermal-hydraulic fields between the N-TH and N-TH-CRUD coupling simulations. (a) The fuel surface temperature with the predicted SNB triggering the surface temperature. (b) Fuel surface heat flux and the predicted earliest and latest occurrence heights of SNB. (c) The coolant temperature.

an average temperature decrease of 1.88 K, with localized differences up to 2.8 K, while the downward power shift enhances power generation and accelerates the temperature rise in the lower fuel segment. Application of the Jens-Lottes boiling heat-transfer correlation given in Eq. (15) reveals that the fuel rod with the lowest power approaches the SNB threshold at 251 cm, whereas the fuel rod with the highest power already exhibits established SNB conditions at 168 cm, demonstrating the strong correlation between the power distribution, SNB initiation, and the CRUD deposition behavior. The axially integrated surface heat-flux profile in Fig. 6(b), obtained from radial integration, predominantly follows the fission power distribution, with a characteristic rise-peak-fall pattern. CRUD effects cause the heat-flux peak to shift upward by approximately 14 cm while increasing the average heat flux by 1618.9 W/m². Notably, the fuel rod with the highest power exhibits a heat flux of 8.7×10^5 W/m² at the SNB location, compared to 7.2×10^5 W/m² for the fuel rod with the lowest power, further highlighting the power-dependent nature of these thermal-hydraulic phenomena. As illustrated in Fig. 6(c), the CRUD-induced power shift leads to elevated coolant temperatures within the (50–300)-cm axial region, exhibiting an average temperature rise of 0.395 K per flow channel. Furthermore, in CRUD-affected fuel assemblies, the coolant outlet temperature of the highest-power rod exceeds that of the lowest-power

rod by 5.8 K, demonstrating the thermal impact of power redistribution. These results underscore how CRUD deposition modifies both the heat-transfer characteristics and the axial power distribution, ultimately influencing key safety parameters such as SNB initiation and peak cladding temperatures.

B. Analysis of CRUD characteristics and mechanism

In Fig. 7, we present the 3D CRUD thickness distribution derived from neutronics-thermal coupling simulations. The spatial distribution [Fig. 7(a)] shows minimal CRUD deposition (0.2–0.3 μ m) in the lower axial region where SNB conditions are absent, with negligible effects on the coolant boron concentration. As the elevation increases, the CRUD deposition initially concentrates in high-power regions, exhibiting both radial expansion and axial variation, while declining in the upper section. The progression is detailed through thickness profiles at four characteristic elevations (190, 230, 270, and 310 cm). In the initial phase [Fig. 7(c1)], CRUD forms preferentially near internal guide tubes, covering 29% of the radial area. Subsequent expansion [Fig. 7(c2)] extends deposition diagonally into medium-power regions (83.3% coverage), followed by diffusion to low-power corners [98.6% coverage; Fig. 7(c3)]. After SNB conditions develop in most regions [Fig. 7(c4)], the radial coverage stabilizes while the average thickness decreases from 34.59 μ m to

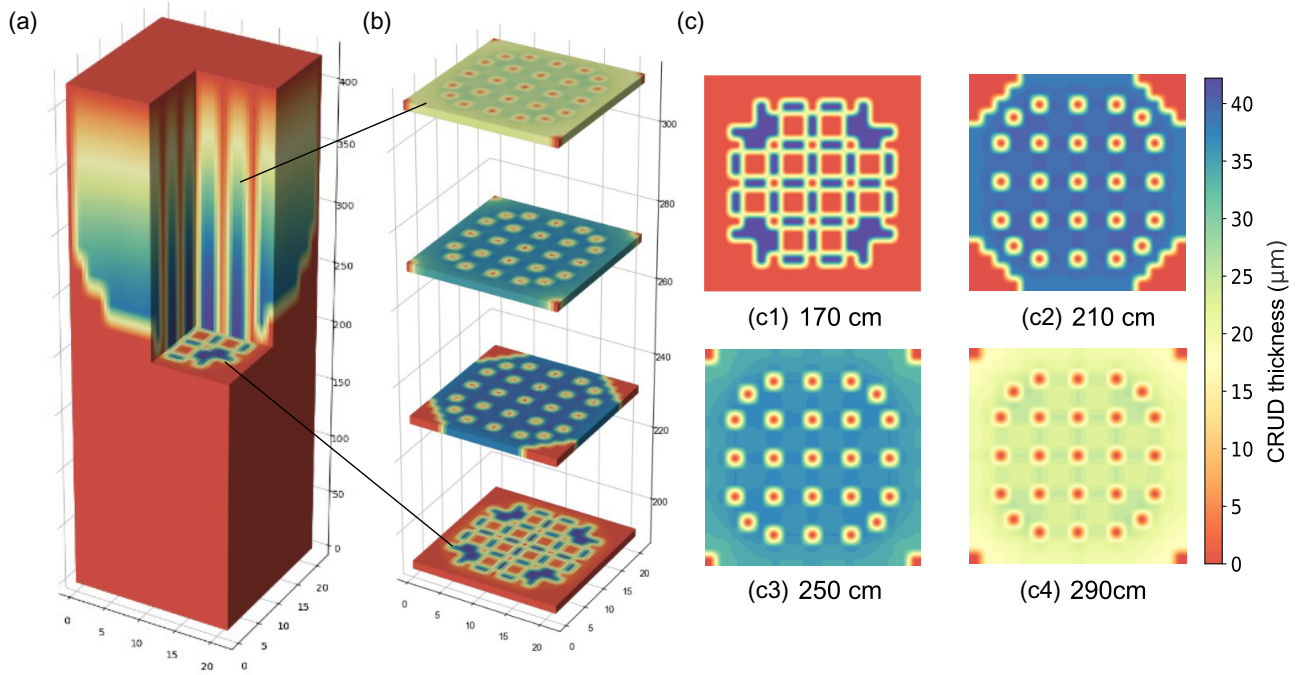


FIG. 7. The CRUD deposition characteristics in the fuel assembly. (a) The 3D distribution of the CRUD thickness. (b) Composite radial distribution of CRUD thickness across axial elevations (170 cm, 210 cm, 250 cm, 290 cm), highlighting progressive expansion from center to periphery and systematic axial attenuation. (c) Localized CRUD thickness at four axial elevations (170 cm, 210 cm, 250 cm, 290 cm), revealing CRUD deposition heterogeneity and peak deposition zones.

26.66 μm , accompanied by a reduction in the internal boron concentration from 0.158 to 0.109 mol/l. Surface heat flux plays a governing role in deposition patterns and composition. Experimental studies [47,48] demonstrate that the CRUD growth thickness varies approximately linearly with the heat flux under isothermal coolant conditions, explaining the observed axial thinning as the heat flux diminishes with the elevation. Notably, corner regions with minimal relative power neither achieve SNB temperatures nor accumulate measurable CRUD. The thickness distribution further reveals localized variations, with guide-tube-adjacent high-power regions exhibiting greater accumulation than diagonally adjacent low-power zones. These observations conclusively link the CRUD deposition dynamics to the geometric configuration and radial power distribution of the assembly.

As shown in Fig. 8, comparative analysis of relative power distributions between fuel rods with the lowest power (without CRUD formation) and the highest power (with extensive CRUD deposition) demonstrates that CRUD-affected assemblies consistently exhibit axial power shifts, regardless of the CRUD accumulation level on individual rods.

Within the same assembly, the AO values show remarkable consistency, with the highest- and lowest-power fuel rods displaying AO values of 6.24% and 6.2%, respectively. Compared to the dashed line representing

the baseline solution without considering CRUD effects, a clear power shift is evident. This observation aligns with documented phenomena [27], where even fresh assemblies adjacent to CRUD-affected ones exhibit AO. The combination of neutron penetrability across the spatial domain and widespread CRUD accumulation leads to reduced neutron flux and power levels at corresponding axial elevations.

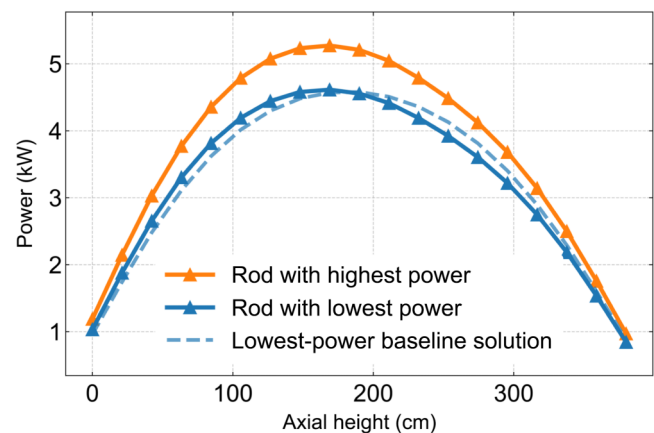


FIG. 8. Neighboring phenomena have been observed in the axial power distributions across individual fuel rods within the assembly. The lowest-power fuel rod, where no CRUD is formed, exhibited almost the same AO as the highest-power fuel rod with extensive CRUD deposition.

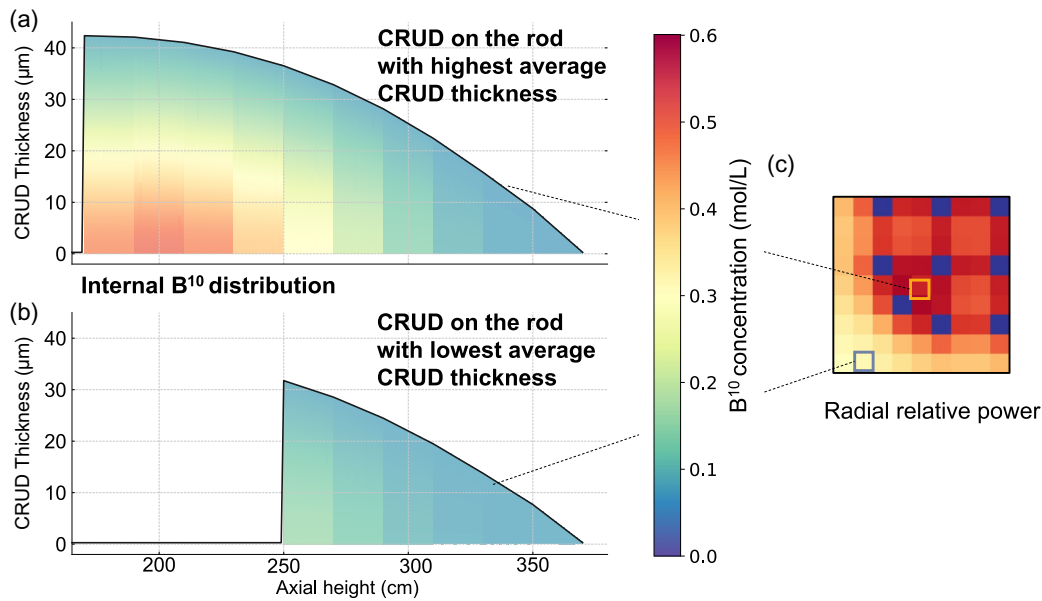


FIG. 9. The axial distribution of the CRUD thickness and the internal boron concentration. (a) A higher average boron concentration is observed not at the SNB initiation point, probably due to enhanced transverse Darcy flow. (b),(c) In most scenarios, both (b) the CRUD deposition thickness and (c) the internal boron accumulation are primarily governed by power and temperature conditions.

Crucially, this “neighboring phenomenon” has significant implications for core-design and fuel-management strategies. Reload core designs need to consider the potential for AO shifts not just in assemblies with high historical CRUD levels but also in neighboring assemblies or even within assemblies containing a mix of CRUD-free and CRUD-bearing rods. This could influence the placement of fresh fuel, burnable poisons, or control-rod patterns to mitigate unexpected power tilts and maintain optimal power shapes throughout the cycle.

Our comprehensive assessment indicates that the axial perturbations induced by the presence of CRUD significantly outweigh the radial effects, manifesting as a global impact on the fuel-assembly power distribution. The overall axial influence is sufficiently pronounced to overshadow any potential axial-distribution variations arising from differing radial power profiles.

In Figs. 9(a) and 9(b), we analyze the CRUD deposition patterns of fuel rods with the highest and lowest average CRUD thickness. As illustrated in Fig. 9(c), they are observed to occur at the locations of both the highest-power and the second-lowest-power fuel rods, demonstrating that the surface heat flux governs both the CRUD growth and composition distribution [47,48]. Elevated heat flux not only increases the CRUD thickness and boron-hideout capacity but also raises internal CRUD temperatures, accelerating chemical reactions and modifying equilibrium constants. Consistent with the literature, localized boron-concentration peaks occur near the fuel surface [33]. However, the highest-power rod in Fig. 9(a) exhibits a distinct behavior at the SNB initiation point: while the CRUD

thickness reaches its maximum, the overall boron concentration is slightly lower than at adjacent axial positions. This phenomenon likely arises from the combined effects of extreme surface heat flux, a substantial CRUD thickness at the SNB point, and pronounced coolant-temperature variations, which enhance transverse Darcy flow within the CRUD. This flow reduces the boron-transport gradient across the deposit, lowering the average concentration—a localized effect driven by the complex interplay of neutronics, thermal hydraulics, and CRUD chemistry. Comparative analysis between Figs. 9(a) and 9(b) further reveals that while CRUD minimally affects global radial power distribution, regional heat-flux variations significantly alter the deposition behavior in individual fuel rods.

IV. CONCLUSIONS

This study develops a high-fidelity multiphysics modeling framework that integrates neutronics, thermal hydraulics, and chemical kinetics to accurately simulate CRUD formation and deposition processes. The computational approach couples these physical domains through an iterative Picard scheme, while implementing a background-mesh methodology to effectively resolve the inherent multiscale nature of CRUD phenomena and ensure numerical accuracy.

A PWR assembly is modeled to conduct steady-state calculations over 180 CRUD deposition days, with the objective of investigating the impact of CRUD on neutron flux, power distribution, and temperature fields, as

well as its associated feedback effects. The analysis reveals that the 3D power distribution within the fuel assembly exhibits significant spatial variations. Under CRUD conditions, the axial power distribution experiences a downward shift of approximately 21 cm toward the lower region of the core, resulting in an axial power offset of approximately 6.27%. In the radial direction, the influence of CRUD on the assembly power is approximately 0.04% of the total power, which is considered negligible in practical terms.

At the individual-fuel-rod level, CRUD induces a proximity effect within the assembly. Even in fuel rods without surface CRUD deposition, nearly identical variations in normalized power distribution are observed, primarily due to axial CRUD accumulation across the entire assembly. Regarding radial effects, the temperature profiles and CRUD characteristics of individual fuel rods exert a negligible influence—less than 0.2%—on their respective axial normalized power distributions.

The coupled effects of the power and temperature fields are the critical factors governing the rapid growth of CRUD—specifically, the onset of SNB. The radial power distribution of fuel within the assembly significantly affects the CRUD deposition patterns and the corresponding internal boron-concentration profile. Furthermore, elevated temperatures, increased power levels, and higher surface heat-flux densities promote enhanced CRUD deposition. An important observation is that high-power conditions intensify transverse Darcy flow within the CRUD, which subsequently reduces the boron-transport gradient across the thickness dimension, leading to a diminished average boron concentration. While CRUD has a negligible impact on the global radial power distribution, localized variations in heat-flux density can significantly alter the CRUD deposition behavior of individual fuel rods.

These findings provide fundamental insights into the complex coupling between the power distribution, SNB, and CRUD formation within PWR fuel assemblies. The results advance our understanding of the governing mechanisms and establish a theoretical foundation for enhancing reactor performance while maintaining stringent operational safety requirements.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data supporting the findings of this study are available within the paper.

APPENDIX A: ASSEMBLY GEOMETRY

VITAS represents a 1/4 symmetry 3D model of a 17×17 PWR assembly that contains 264 fuel rods and 25 guide tubes. The model has an active fuel height of 380 cm and 20 cm of water-reflector layers at both ends, with vacuum boundary conditions at the ends of the reflectors. For the thermal-hydraulic calculation, the assembly model is initialized with a coolant inlet temperature of 565 K and an inlet mass flow rate of 24.056 kg/s, operating under a pressure condition of 15.5 MPa. Each fuel pin is discretized into ten radial meshes to capture detailed spatial variations and the heat conduction across the gas gap is explicitly

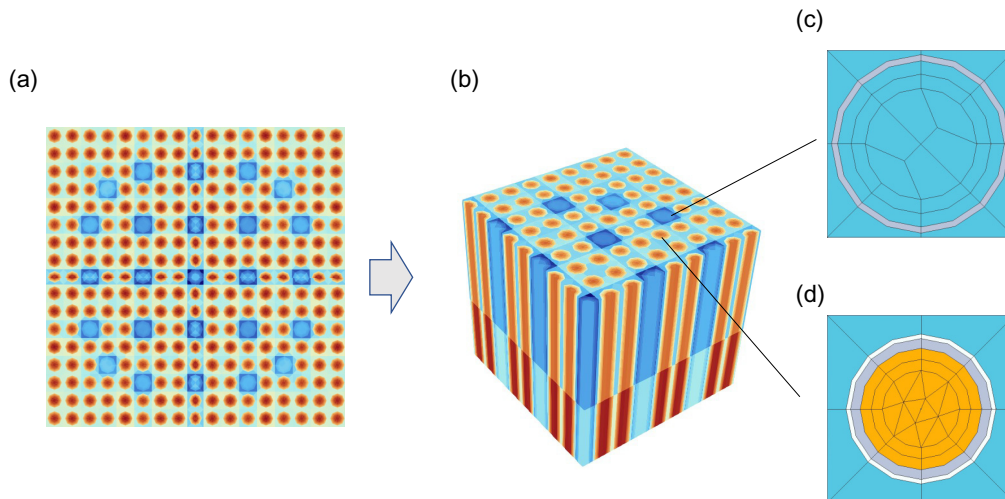
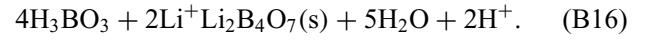
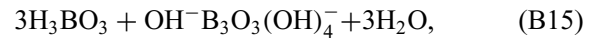
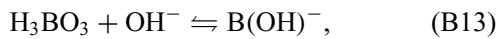
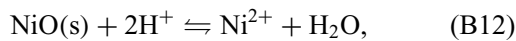
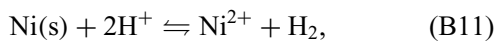
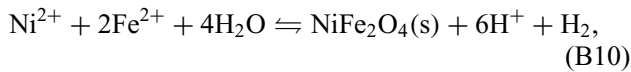
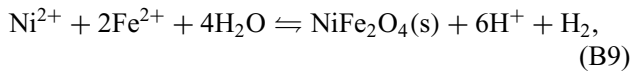
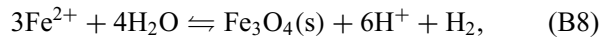
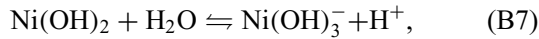
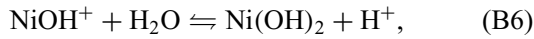
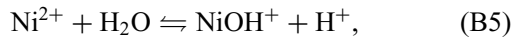
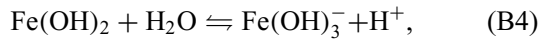
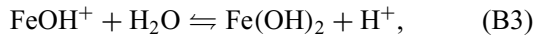
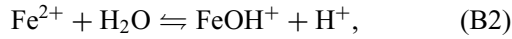
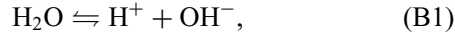


FIG. 10. (a),(b) The (a) global cell arrangement within the (b) assembly. (c) The unstructured mesh of guide tubes. (d) Fuel-rod unstructured meshes: the white radial regions are designed to acquire background CRUD and coolant nuclide density.

accounted for in the model. In the study, the CRUD conditions of a PWR after continuous operation for 180 days have been simulated, with the boron concentration in the coolant set to 1300 ppm.

APPENDIX B: CHEMICAL-EQUILIBRIUM EQUATIONS

The chemical-equilibrium equations considered in the CRUD model are as follows:



- [1] S. Chu and A. Majumdar, Opportunities and challenges for a sustainable energy future, *Nature* **488**, 294 (2012).
- [2] C. Karakosta, C. Pappas, V. Marinakis, and J. Psarras, Renewable energy and nuclear power towards sustainable development: Characteristics and prospects, *Renewable Sustainable Energy Rev.* **22**, 187 (2013).
- [3] J. R. Lovering, A. Yip, and T. Nordhaus, Historical construction costs of global nuclear power reactors, *Energy Policy* **91**, 371 (2016).
- [4] E. Severnini, Impacts of nuclear plant shutdown on coal-fired power generation and infant health in the Tennessee Valley in the 1980s, *Nat. Energy* **2**, 1 (2017).
- [5] L. M. Freese, G. P. Chossière, S. D. Eastham, A. Jenn, and N. E. Selin, Nuclear power generation phase-outs redistribute US air quality and climate-related mortality risk, *Nat. Energy* **8**, 492 (2023).
- [6] P. Fernández-Arias, D. Vergara, and J. A. Orosa, A global review of PWR nuclear power plants, *Appl. Sci.* **10**, 4434 (2020).
- [7] S. Chen, T. Wang, Z. Zhang, R. Li, S. Yuan, R. Zhang, C. Yuan, C. Zhang, and J. Zhu, Linear regression and machine learning for nuclear forensics of spent fuel from six types of nuclear reactors, *Phys. Rev. Appl.* **19**, 034028 (2023).
- [8] J. de Dios Sánchez, Key Emerging Issues and Recent Progress Related to Plant Chemistry/Corrosion (PWR, CANDU, and BWR Nuclear Power Plants), Tech. Rep. (Advanced Nuclear Technology International, 2024).
- [9] F. Cattant, D. Crusset, and D. Féron, Corrosion issues in nuclear industry today, *Mater. Today* **11**, 32 (2008).
- [10] P. M. Scott and P. Combrade, in *Corrosion: Environments and Industries*, edited by S. D. Cramer and B. S. Covino, Jr. (ASM International, Materials Park, OH, 2006), Vol. 13C, p. 0.
- [11] J. Buongiorno, Can corrosion and CRUD actually improve safety margins in LWRs? *Ann. Nucl. Energy* **63**, 9 (2014).
- [12] J. Deshon, D. Hussey, B. Kendrick, J. McGurk, J. Secker, and M. Short, Pressurized water reactor fuel crud and corrosion modeling, *JOM* **63**, 64 (2011).
- [13] R. Riess, Chemistry experience in the primary heat transport circuits of Kraftwerk Union pressurized water reactors, *Nucl. Technol.* **29**, 153 (1976).
- [14] H. Fenech, *Heat Transfer and Fluid Flow in Nuclear Systems* (Pergamon Press Inc., Oxford, U.K, 1981).
- [15] J. Breitenbach, I. V. Roisman, and C. Tropea, Drop collision with a hot, dry solid substrate: Heat transfer during nucleate boiling, *Phys. Rev. Fluids* **2**, 074301 (2017).
- [16] Y. Hao, Y. Zhang, and A. Prosperetti, Mechanics of gas-vapor bubbles, *Phys. Rev. Fluids* **2**, 034303 (2017).
- [17] Y. Liu, X. Liu, T. Zhang, and H. He, Understanding flow fouling deposition and solute hideout–return behavior at the phase change interface, *ACS Appl. Mater. Interfaces* **16**, 4719 (2024).

- [18] F. D. Nicholson and J. V. Sarbutt, The effect of boiling on the mass transfer of corrosion products in high temperature, high pressure water circuits, *Corrosion* **36**, 1 (1980).
- [19] J. Yang, J. Wang, J. Liu, S. Wang, D. Yun, D. Ma, Y. Li, and D. Xu, Microstructural understanding on the fouling behavior of crud on PWR fuel cladding surface, *J. Nucl. Mater.* **582**, 154500 (2023).
- [20] W. A. Byers, G. Wang, M. Y. Young, and J. Deshon, Simulation of PWR CRUD, in *International Conference on Nuclear Engineering* (2014), Vol. 1, p. V001T02A029.
- [21] R. A. Castelli, *Nuclear Corrosion Modeling: The Nature of CRUD* (Butterworth-Heinemann, Oxford, U.K., 2010).
- [22] M. Barton, M. R. Conqueror, K. Garbett, M. A. Mantell, M. E. Phillips, M. V. Polley, and W. A. Westall, in *Water Chemistry of Nuclear Reactor Systems 8* (Thomas Telford Publishing, London, England, 2001), pp. 2: 391–398.
- [23] Y. Liu, H. He, T. Zhang, and X. Liu, Pressurized water reactor fuel corrosion-related unidentified deposit and its related safety issues—I. Corrosion product deposition and heat transfer, *Ann. Nucl. Energy* **208**, 110758 (2024).
- [24] M. P. Short, D. Hussey, B. K. Kendrick, T. M. Besmann, C. R. Stanek, and S. Yip, Multiphysics modeling of porous CRUD deposits in nuclear reactors, *J. Nucl. Mater.* **443**, 579 (2013).
- [25] J. Pongpuak, Ph.D. thesis, Department of Chemical Engineering, University of New Brunswick, 2006.
- [26] P. Cohen, Heat and mass transfer for boiling in porous deposits with chimneys, *AIChE Symp. Ser.* **70**, 71 (1974).
- [27] J. Deshon, PWR axial offset anomaly (AOA) guidelines, revision 1, EPRI (Palo Alto, CA, 2004), <https://www.epri.com/research/products/00000000001008102>.
- [28] L. Zou, H. Zhang, J. Gehin, and B. Kochunas, Coupled thermal-hydraulic/neutronics/CRUD framework in prediction of CRUD-induced power shift phenomenon, *Nucl. Technol.* **183**, 535 (2013).
- [29] EPRI, Boron-Induced Offset Anomaly (Palo Alto, CA, 2017), Software No. 3002012131, <https://www.epri.com/research/products/000000003002012131>.
- [30] G. Wang, P. Sapienza, R. J. Fetterman, M. Y. Young, J. R. Secker, S. W. Nelson, R. L. Oelrich, and Y. Sung, in *Volume 3: Thermal-Hydraulics; Turbines, Generators, and Auxiliaries* (American Society of Mechanical Engineers, Anaheim, California, 2012), pp. 93–101.
- [31] B. Collins, J. Galloway, R. Salko, Jr., K. Clarno, A. Wysocki, B. Okhuysen, and A. D. Andersson, Whole core CRUD-induced power shift simulations using VERA, Tech. Rep. (Oak Ridge National Laboratory (ORNL), Oak Ridge, Tennessee, 2018).
- [32] D. J. Walter, B. K. Kendrick, V. Petrov, A. Manera, B. Collins, and T. Downar, Proof-of-principle of high-fidelity coupled CRUD deposition and cycle depletion simulation, *Ann. Nucl. Energy* **85**, 1152 (2015).
- [33] M. Jin and M. Short, Multiphysics modeling of two-phase film boiling within porous corrosion deposits, *J. Comput. Phys.* **316**, 504 (2016).
- [34] S. Seo, B. Park, S. J. Kim, H. C. Shin, S. J. Lee, M. Lee, and S. Choi, BOTANI: High-fidelity multiphysics model for boron chemistry in CRUD deposits, *Nucl. Eng. Technol.* **53**, 1676 (2021).
- [35] Y. Liu, J. Chen, G. Wang, H. He, T. Zhang, and X. Liu, Pressurized water reactor fuel corrosion-related unidentified deposit and its related safety issues—II. Corrosion product deposition and heat transfer modeling, *Ann. Nucl. Energy* **211**, 110932 (2025).
- [36] H. G. Joo, J. Y. Cho, K. S. Kim, C. C. Lee, and S. Q. Zee, *Methods and Performance of a Three-Dimensional Whole-Core Transport Code DeCART* (American Nuclear Society, Chicago, Illinois, 2004).
- [37] T. Zhang, W. Xiao, H. Yin, Q. Sun, and X. Liu, VITAS: A multi-purpose simulation code for the solution of neutron transport problems based on variational nodal methods, *Ann. Nucl. Energy* **178**, 109335 (2022).
- [38] T.-I. Hu, H.-c. Wu, L.-z. Cao, Y.-q. Zheng, and K. Zhuang, Neutronics and thermal-hydraulics coupling analysis of molten salt reactor at steady state, *At. Energy Sci. Technol.* **10**, 1823 (2016).
- [39] J. Tang, M. Huang, Y. Zhao, X. Ouyang, and J. Huang, A new procedure for solving steady-state and transient-state nonlinear radial conduction problems of nuclear fuel rods, *Ann. Nucl. Energy* **110**, 492 (2017).
- [40] W. Jens and P. Lottes, *Analysis of Heat Transfer, Burnout, Pressure Drop and Density Data for High-Pressure Water* (Naval Reactor Division, Argonne National Laboratory, Lemont, IL, 1955).
- [41] C. Pan, B. G. Jones, and A. J. Machiels, Concentration levels of solutes in porous deposits with chimneys under Wick boiling conditions, *Nucl. Eng. Des.* **99**, 317 (1987).
- [42] C. B. Lee, Ph.D. thesis, Modeling of corrosion product transport in PWR primary coolant, Department of Nuclear Engineering, Massachusetts Institute of Technology, 1990.
- [43] C. Y. Tai and C.-H. Lin, Crystal growth kinetics of the two-step model, *J. Cryst. Growth* **82**, 377 (1987).
- [44] B. G. Park, S. Seo, S. J. Kim, J. H. Kim, and S. Choi, Meso-scale multi-physics full coupling within porous CRUD deposits on nuclear fuel, *J. Nucl. Mater.* **512**, 100 (2018).
- [45] R. Macfarlane, D. W. Muir, R. M. Boicourt, A. C. Kahler, and J. L. Conlin, *The NJOY nuclear data processing system, version 2016*. Los Alamos National Lab. (LANL), Los Alamos, NM (United States, 2017).
- [46] J. A. Turner, K. Clarno, M. Sieger, R. Bartlett, B. Collins, R. Pawlowski, R. Schmidt, and R. Summers, The virtual environment for reactor applications (VERA): Design and architecture, *J. Comput. Phys.* **326**, 544 (2016).
- [47] Y. Liu, G. Wang, H. He, T. Zhang, and X. Liu, Pressurized water reactor fuel corrosion-related unidentified deposit and its related safety issues—III. N-TH-M coupled CIPS prediction, *Ann. Nucl. Energy* **208**, 110800 (2024).
- [48] S. H. Baek, H.-S. Shim, J. G. Kim, and D. H. Hur, Effects of heat flux on fuel crud deposition and sub-cooled nucleate boiling in simulated PWR primary water at 13 MPa, *Ann. Nucl. Energy* **133**, 178 (2019).