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Coupled Simulation of CRUD Growth in PWRs Using a Time-Dependent CRUD Source Term Model

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1. Introduction

The formation of CRUD on fuel surfaces in pressurized water reactors (PWRs) is not solely determined by in-core operating conditions; rather, they heavily depend on the temporal evolution of the morphology and physical quantity of corrosion products entering the core. Therefore, accurately understanding the core inlet source term, which is the cumulative result of various physicochemical processes occurring throughout the primary coolant system, is essential for elucidating the behaviors of CRUD.

The developmental process of CRUD originates from metallic corrosion and the formation of inner oxide layers on the surfaces of primary system components, such as the Steam Generator (SG), Hot Leg (HL), and Cold Leg (CL). The resulting corrosion products are either released into the coolant as ions or form outer oxide layers and particulate species, which are then transported throughout the system. During this transport, the corrosion products undergo complex interactions where they are continuously deposited onto the system surfaces or, conversely, eroded by the coolant flow and released back into the coolant. The cumulative result of these deposition and erosion behaviors within the system is the key factor governing the time-dependent variation of the particle concentration entering the core.

Reflecting this life-cycle perspective of CRUD, the present study proposes a control-volume-based mass balance model that calculates the time-varying core inlet source term by incorporating the deposition and erosion mechanisms of corrosion products throughout the entire primary system [1]. Furthermore, by coupling the calculated core inlet conditions with a CRUD growth analysis code, this study aims to establish an integrated analytical framework capable of quantitatively evaluating the effects of the time-varying source term on CRUD growth.

2. Methods and Results

This section describes the configuration and governing equations of a system-partitioned mass balance model, which was developed to calculate the dissolved and particulate behaviors of corrosion products in the primary coolant system of a pressurized water reactor (PWR). An independent code was developed to simulate the generation and accumulation of CRUD source terms within the primary circuit, with physical models and theoretical framework based on the CASL technical report [1]. Furthermore, it details the mathematical implementations and numerical solution procedures for the supporting sub-modules that simulate water chemistry, corrosion, precipitation and nucleation, erosion, and thermal-hydraulics.

2.1 Formulation of the PWR CRUD Source Term Model

The CRUD source term model developed in this study was implemented in Python. It calculates the temporal evolution of dissolved and particulate corrosion product concentrations by coupling a control-volume-based mass balance model—which partitions the primary coolant system into representative segments (steam generator, cold leg, hot leg, fuel, and core)—with segment-wise sub-modules for water chemistry, precipitation, and erosion. Time integration is performed by constructing a system of coupled ordinary differential equations (ODEs) for the key state variables of each segment, including dissolved concentration, particulate concentration, and the accumulated inventory of surface deposit layers. The numerical procedure proceeds as follows: constructing convective transport terms between segments based on the prescribed flow and volume conditions; evaluating the source/sink terms (release, precipitation, deposition, and erosion) by reflecting the thermodynamic solubility in real-time through the water chemistry sub-module based on the local temperature and pH conditions of each segment; and numerically integrating the combined ODE system. The governing equation for the dissolved species concentration $C_{s,i}$ in each segment i is expressed in the form of mass conservation as follows [2]:

$$M_i \frac{dC_{s,i}}{dt} = \dot{m}_{i-1\rightarrow i} C_{s,i-1} - \dot{m}_{i\rightarrow i+1} C_{s,i} + S_i^{rel} - S_i^{prec} \quad (1)$$

where M_i is the coolant mass within the segment, $\dot{m}$ is the mass flow rate between segments, S_i^{rel} is the release term of dissolved species from the surface into the coolant, and S_i^{prec} is the precipitation loss term converting dissolved species into particulates.

An identical transport equation format is applied to the particulate concentration $C_{p,i}$. However, for particulates, additional terms are considered, including a generation term due to precipitation(S_i^{prec}), a loss term due to surface deposition(S_i^{depo}), and a generation term due to erosion(S_i^{eros}), which can be expressed as follows:

$$M_i \frac{dC_{p,i}}{dt} = \dot{m}_{i-1\rightarrow i} C_{p,i-1} - \dot{m}_{i\rightarrow i+1} C_{p,i} + S_i^{prec} - S_i^{depo} + S_i^{eros} \quad (2)$$

2.2 Corrosion Product Generation and Behavior Model

In this study, the CRUD source term is modeled as a sequence of mechanisms comprising corrosion growth, dissolved ion release, particle formation, deposition, and erosion. Each stage is directly linked to the corresponding source and sink terms in the system-partitioned mass balance equations.

Corrosion growth is described by the parabolic growth behavior of the inner oxide layer thickness x [1]:

$$\mathrm{x(t)} = \frac{k_p(T)\sqrt{t}}{\rho_{oxide}} \quad (3)$$

where x is the film thickness, k_p is the corrosion rate constant, ρ_{oxide} is the oxide density.

Release is defined as the supply of dissolved ions, which is limited by the inner oxide layer. It is formulated such that the release rate decreases as the oxide layer thickness increases, reflecting the increased mass transfer resistance [1]:

$$\mathrm{R} = \frac{D_{oxide,GB}^{Ni} \rho_{alloy} wt\%}{x(t)} \times A_{cell} \quad (4)$$

where R is the corrosion release rate, $D_{oxide,GB}^{Ni}$ is the nickel diffusion coefficient in the grain boundary of the inner oxide, ρ_{alloy} is the alloy density, wt% is the weight fraction of the element Ni and Fe in the alloy, A_{cell} is the surface area of the cell.

Particle formation is driven by precipitation, which depends on the thermodynamic saturation state of the coolant. The Gibbs free energy of the reaction(ΔG_{rxn}) for this state is evaluated as follows [3]:

$$\Delta G_{rxn} = \Delta_f G^{\circ}_{NiFe_2O_4}(T) + \mu_{H_{2(aq)}}(T) - \mu_{Ni^{2+}(aq)}(T) - 2\mu_{Fe^{2+}(aq)}(T) - 4\mu_{H_2O}(T) \quad (5)$$

where ΔG_{rxn} is the Gibbs free energy change of the reaction, $\Delta_f G^{\circ}_{NiFe_2O_4}(T)$ is the Gibbs free energy of formation of $NiFe_2O_4$, and $\mu_i(T)$ denotes the chemical potential of aqueous species i.

The surface deposit inventory is modelled by a local mass balance, where precipitation adds material and flow-assisted detachment removes it:

$$\frac{dW}{dt} = R_{precip} - k_e W \quad (6)$$

where W is the surface-deposited particulate mass, R_{precip} is the precipitation rate, and k_e is the erosion rate coefficient.

The formed particles deposit onto surfaces to form an outer oxide layer. Subsequently, under the prevailing flow and thermal-hydraulic conditions, this layer undergoes erosion, releasing particles back into the coolant. In this model, the particle detachment probability (p) is formulated as a combined effect of dehydration and surface–particle interactions [4]:

$$p = p_1(dehydration) \times p_2(surface - particle\ interaction) \quad (7)$$

The erosion rate constant (k_e) for particle release is defined as [4]:

$$k_e = \frac{\gamma k_c}{k_c + p(v_B + v_f)} \quad (8)$$

where k_e is erosion rate coefficient, γ is the release coefficient, k_c is the mass transfer coefficient, v_B is the particle velocity by Brownian motion, v_f is the particle velocity by fluid flow.

2.3 Coupling with the CRUD Growth Analysis Code and Results

Applying the CRUD source term model developed in this study, the core-inlet concentrations of total dissolved Fe and Ni were preliminarily calculated to range from approximately 3.01 to 3.09 ppb and 0.217 to 0.228 ppb, respectively, over the operational cycle. The particulate concentrations converged to stable levels following an initial transient behavior and were evaluated at approximately 0.02 ppb and 0.04 ppb for Fe and Ni, respectively, at the end of the cycle. Dissolved–particulate partitioning is resolved using a finite-rate kinetic formulation. Therefore, the near-flat dissolved trends likely indicate rapid attainment of a dynamic steady state.

To ensure the reliability of these preliminary results, future work will focus on quantitatively validating the source term predictions against long-term operational data from commercial pressurized water reactors (PWRs). Furthermore, a sensitivity analysis will be conducted to evaluate how variations in water chemistry operating conditions affect the core inlet concentrations.

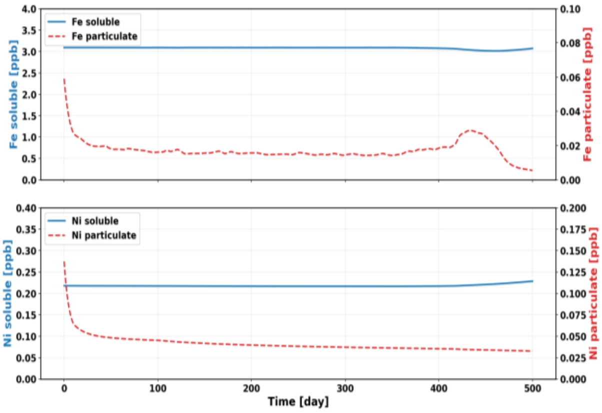

Fig. 1. Time-dependent evolution of soluble and particulate Fe and Ni concentrations at the core inlet.

The derived time-dependent core inlet conditions were directly coupled to the CRUD growth analysis code on the same time grid. Compared to the existing model input, applying this time-dependent Fe/Ni input generally increased the CRUD thickness across the entire axial length. This occurred because the system model maintained higher soluble species concentrations at the core inlet. Consequently, the time-dependent input increased the CRUD thickness by approximately 10–20 μm in most axial regions compared to the existing model input.

The overall shape of the axial thickness distribution remained qualitatively similar in both cases. However, the increase in thickness obtained with the model-derived Fe/Ni input was smaller in the peak-thickness zone (approximately H = 2.2–2.9 m, where the axial profile reaches its maximum) than in the lower-to-mid elevations (H < ~2.0 m). The cause of this difference in sensitivity depending on the axial position needs to be quantitatively identified in future studies.

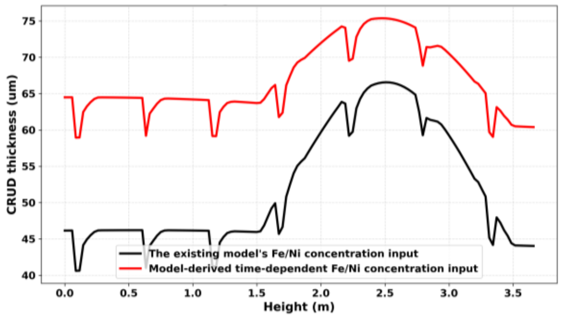

Fig. 2. Comparison of CRUD thickness distribution along the axial height: Results of applying the existing model input versus the source term model-derived Fe/Ni input. (For the baseline case, the axial CRUD thickness profile was obtained using the model reported in Ref. [5])

3. Conclusions

This study formulated a system-partitioned mass balance model to evaluate the time-dependent behavior of the CRUD source term in a pressurized water reactor (PWR) primary coolant system, proposing an integrated analytical framework that couples this model with CRUD growth analyses. The model calculates the temporal evolution of Fe/Ni concentrations at the core inlet through a series of sequential mechanisms ranging from corrosion growth, release, and precipitation and dissolution to deposition and erosion.

Preliminary results from the coupled analysis confirmed that applying the time-dependent Fe/Ni input increases the CRUD thickness across the entire axial length compared to the input of the existing model. This is interpreted as the effect of differences in soluble concentration levels altering the net deposition. On the other hand, the increase in thickness near the peak region (H ≈ 2.2–2.9 m) was relatively smaller than in other regions.

Future work will focus on securing the predictive accuracy of the source term model through quantitative cross-validation with long-term operational data from commercial PWRs, and systematically analyzing the causes of the localized CRUD growth behavior observed in the axial peak region. Ultimately, based on these efforts, the research will be expanded to the optimization of water chemistry operational guidelines to minimize in-core CRUD growth.

Acknowledgements

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