Dissertation title: Improving Modeling of Corrosion Products (CRUD) in the Pressurized Water Reactors through the Experimental Determination of CRUD Characteristics

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Abstract

Corrosion products such as nickel-iron spinel oxides (known as CRUD) in the coolant circuits of pressurized water (PWR) reactors may lead to particulate fouling, negatively impacting power distribution and changing local chemistry. The transport and deposition of particles depend in part on the surface charge of the particles and the nearby surfaces. Tuning coolant chemistry and the composition of the primary circuit materials has been used as an empirical lever for crud mitigation, but experimentation is limited. This work aims to build a physics-based CRUD deposition model. The model will predict deposition in environments and geometries representative of coolant circuits of PWRs, and the main goal is to understand the role of water chemistry parameters, the effect of Ni composition, Zn addition, and reducing agents on the CRUD deposition.

To ensure the relevance of this model, the surface properties of CRUD particles have been measured and incorporated into simulations to study the impact of the parameters that are affected by water chemistry. To this end, a library of particles, specifically the nickel-zinc-iron spinel oxides ternary system, has been synthesized, covering a range of compositions and water chemistry (Zn addition, and reducing environment). Similarly, stainless steel coupons were exposed to hydrothermal conditions to understand the growth and possible detachment of nanoparticles from these surfaces. Surface characterizations were performed on the single-phase ferrite nanoparticles to obtain Isoelectric Point (IEP). Increasing Nickel content shifted surfaces toward a more basic character. Higher concentrations of Zinc shifted the surface towards more acidic character, effectively lowering the IEP.

To simulate the transport and deposition process of CRUD particles, a COMSOLTM simulation was designed. To account for the differing length and time scales of the physical processes involved, sequential multiscale modeling was implemented. A macroscale model solves the fluid flow and particle trajectories and is later coupled with a fine-scale particle adhesion model. The overall probability of deposition was obtained by combining the results from macro-scale simulations and the fine scale simulations. The smaller particles (< 500 nm) followed a nearly

digital response to the value of the Stern potential, while the larger particles had relatively slow decay with increasing Stern potential.

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