Multi-layer Modeling of Zirconium Clad Corrosion during Pre- and Post- Transition Regimes

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Abstract

We develop a multi-layer model for predicting the high-temperature corrosion of zirconium before the formation of cracks. The model includes the formation of two oxide sub-layers on the metal clad, whose interfaces are tracked using a coupled diffusion-reaction model. The temperature dependency and thermomigration is central in our model, where the charge distribution in the vicinity of the corrosion interface hinders the corrosion rate which has been approximated with the a third power law with time.

For bridging the two corrosion regime during the transition, we develop an analytical criterion based on compressive yielding of the oxide as an expitaxial layer adjacent to the metal, where the percolation threshold for the cracked medium has been achieved. We develop a new constriction-based percolation paradigm, using cellular automata to predict the transport of oxygen through a stochastically-cracked Zr oxide layer in real-time. We simulate such branching trees by generating a series of porosity-controlled media. Consequently, our model predicts the arrival rate of oxygen ions at the oxide interface during the post-transition regime, where the bulk diffusion is no longer the rate-limiting factor.

Keywords: zircaloy clad, percolation, corrosion cracking, zirconium oxidation, nuclear reactor.

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