

## Thermodynamic Modeling of the Adsorption of Boric Acid on Fuel Crud Deposit from the Pressurized Water Reactors

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The adsorption of boric acid on porous fuel crud deposit in the primary water circuits of pressurized water reactors (PWR) has been believed to play an important role in the accumulation of boron in the deposits [1]. The formation and presence of boron adsorbed deposit in certain parts of the circuit can lead to a down-rating of the plant and partially results in the phenomenon known as Axial Offset Anomaly (AOA) [2]. In order to understand the chemical and physical process of the adsorption and to develop a strategy to mitigate boron accumulation and avoid the AOA, it is necessary to study the adsorption process at water-solid interface and develop a comprehensive chemistry model, which can represent and predict the adsorption phenomenon in a relevant broad range of pH and temperature.

A comprehensive surface complexation model has been developed to study the adsorption process at water-solid interface by combining the diffuse layer model [3], which explicitly takes into account the effect of the surface charge and surface potential on the adsorption, and the mixed-solvent electrolyte model [4], which provides an accurate and comprehensive description of the speciation of boron and lithium aqueous solution, and makes it possible to account for the pH effect on the adsorption. In all examined cases, the model is shown a good agreement with temperature-dependent, pH-dependent and boron concentration-dependent experimental data. The model provides good estimations and predictions for the boron adsorption on magnetite and  $ZrO_2$  as a function of temperature, especially at elevated temperature. The model predicts that the adsorbed amount of boron on  $ZrO_2$  increases as temperature increases and reaches the maximum at temperature 175 °C, and then decreases as temperature increases. The zero point of charge at room temperature could be accurately calculated with the model. The approach presented in this work can be generalized to study the surface complexation adsorption at solid-liquid surface.

### References

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