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Bringing machine learning into modeling of solid-solution interactions

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Surface complexation models are developed to simulate solid-solution interactions of minerals and ligands integrating surface chemistry parameters and account for various environmental conditions. Simulation of adsorption processes have been traditionally approached through laboratory studies and surface complexation modeling simulations to fit experimental data. Interdependency associated with physicochemical parameters and the impact of the surface structure on ligand adsorption highly contributes to the variability of the simulation and thermodynamic parameters extracted from the simulations. The RES^{3}T Rossendorf Expert System for Surface and Sorption Thermodynamics maintains a database with thermodynamic parameters accumulating literature data from the past three decades. Previous approaches have explored the potential of unifying parameters to simulate multiple adsorption datasets with the goal of facilitating the application surface complexation modeling in the field. However, thermodynamic parameters do not converge to single values as site denticity effects and differences between energetically favorable sites contribute to variable parameters. This presentation explores the application of machine learning into surface complexation modeling to compare deterministic with probabilistic findings in surface complexation parameters. Supervised machine learning approaches including random forest, gradient boosting, and neural network are utilized to compare fitted surface complexation parameters. The discussion will also expand to exploring if this approach can yield meaningful connections to mechanistic phenomena.