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From Deterministic to Probabilistic Frameworks in Reactive Transport Modeling

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Modeling contaminant fate in groundwater is a critical priority in environmental engineering. Reactive transport models that incorporate solid-solution interactions offer a more robust and accurate approach to predicting contaminant sorption mechanisms, improving our ability to model the fate and transport of contaminants in groundwater compared to conventional models. In contrast to the conventional approach where the solid-water partition coefficient (Kd) is used to quantify the adsorption of various ligands, the mechanistic description of surface equilibria integrated molecular-based information (surface species and binding mechanisms, chemical reactions, thermodynamic parameters and mass and charge balances has been approached through surface complexation models (SCMs) [1,2]. Surface complexation models (SCMs) offer several advantages, as they account for environmental and integrate spectroscopic evidence. However, a major challenge remains: the thermodynamics of sorption reactions are highly sensitive to environmental conditions and the inherent heterogeneity of subsurface conditions. The spatial and temporal variability in large-scale transport systems adds significant complexity, which often limits the predictive capabilities of reactive transport models.

The study will showcase the sensitivity and uncertainty analyses to quantify the impact of parameter variability on long-term model predictions and to identify critical factors influencing system behavior in mineral-solution interactions. Stochastic simulation techniques, such as Gaussian random field generation and other probabilistic frameworks are applied to simulate the impact of the variability in surface complexation equilibrium parameters. These stochastic model outputs are compared to deterministic simulations to assess the influence of heterogeneity on predicted contaminant transport and transformation behavior. This research will advance the fundamental understanding of the thermodynamic mechanisms governing contaminant sorption across heterogeneous mineral-ligand systems and it will produce a robust dataset linking laboratory-derived parameters to field-scale processes.

References

[1] Davis, Meece, Kohler & Curtis (2004), *Geochimica et Cosmochimica Acta 68* (18), 3621–3641.

[2] Hiemstra & Van Riemsdijk (1996), *Journal of Colloid and Interface Science 179* (2), 488–508.