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Advancing Reactive Transport Simulations: The Impact of Advective/Diffusive Mineral Accessibility in Sandstones

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Reactive transport simulations play a crucial role in advancing our understanding of geochemical subsurface processes, such as modeling geological carbon sequestration and hydrogen storage. These simulations typically employ mass conservation equations to represent chemical reactions and transport phenomena in porous media, which can occur through dispersive/diffusive or advective mechanisms. The accuracy of these simulations depends on our understanding of fundamental formation properties, including mineral abundance, pore structure, porosity, and accessible surface area (ASA). As reactive fluids flow through interconnected pores, they interact with accessible mineral surfaces either advectively (via macropores) or diffusively (through nanopores in the clay pore network). These interactions are referred to here as advective and diffusive accessibility. Variations in accessibility can result in different reaction rates on mineral surfaces. To incorporate these variations into the model, the dispersion-diffusion tensor (D) is modified by adjusting the tortuosity (τ). The main outcomes of this study include quantifying the advective and diffusive accessibility for each mineral phase and developing a correction factor for dispersion-diffusion tensor based on clay type and thickness. These corrections are intended to improve the predictive capabilities of reactive transport models in geological studies. Using Scanning Electron Microscopy Backscattered Electron (SEM-BSE) images, processed mineral maps, and connectivity maps from previous research, diffusive and advective accessibility is determined by counting accessible mineral pixels adjacent to connected nanopores or macropores. The tortuosity value is then adjusted based on the quantified advective and diffusive accessibility for each mineral phase, along with measured clay coating thickness and clay type. Finally, simulations are compared to evaluate the impact of these modifications.

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References

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