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Reactive transport modeling in aqueous environments using the Nernst–Planck formulation

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Water in natural environments consists of many ions, which exert electric forces on each other. We discuss whether the coulombic effects are relevant in describing mixing and reaction processes in natural environments or laboratory experiments. A typical model for electric interactions in dilute aqueous solutions is the Nernst–Planck equation.

Using FEniCS (fenicsproject.org) and Reaktoro (reaktoro.org), we solve the Nernst–Planck transport and equilibrium reactions of the ionic species in water. By comparing numerical simulations to reaction-driven flow experiments performed in a Hele-Shaw cell, we show that the electric interactions between ions can be relevant in mixing and reaction processes. We further discuss the numerical techniques in solving the Nernst–Planck system. In microfluidic experiments considering the mixing of aqueous fluids or electrokinetic effects, the Nernst–Planck equation can be essential to describe fluids' behavior.

Participation

In-Person

References

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