Simulation of electric charge in the electrolysis of electrolyte solution using particle technique

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Abstract: This study presents a particle-based simulation framework for modeling charge dynamics during the electrolysis of electrolyte solutions. Traditional continuum models often fail to capture the discrete interactions and stochastic behavior of ions at the microscale. To address this, we employ a particle technique where each ion is treated as a charged particle governed by electrostatic forces, Brownian motion, and applied electric fields. The simulation incorporates ion migration, diffusion, and recombination reactions within a defined computational domain. By tracking individual particle trajectories, the model accurately reproduces concentration gradients, double-layer formation, and current-voltage characteristics. Validation against analytical solutions and experimental data for simple binary electrolytes demonstrates strong agreement. The results highlight the method's ability to resolve local charge imbalances and transient phenomena that are critical for optimizing electrochemical processes. This approach offers a versatile tool for studying complex electrolyte systems, providing insights into electrode kinetics and mass transport limitations. The framework can be extended to multi-ion systems and porous electrode geometries, advancing the design of electrochemical cells and energy storage devices.

Keywords: particle simulation, electrolysis, electrolyte solution, electric charge