Modeling Electric Double-Layers Including Chemical Reaction Effects

A physicochemical and numerical model for the transient formation of an electric double-layer between an electrolyte and a chemically-active flat surface is presented, based on a finite elements integration of the nonlinear Nernst-Planck-Poisson model including chemical reactions. The model works for symmetric and asymmetric multi-species electrolytes and is not limited to a range of surface potentials. Numerical simulations are presented, for the case of a CaCO3 electrolyte solution in contact with a surface with rate-controlled protonation/deprotonation reactions. The surface charge and potential are determined by the surface reactions, and therefore they depend on the bulk solution composition and concentration.

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