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Titel des Beitrags: A 3D finite element approach for the coupled numerical simulation of electrochemical systems and fluid flow
Abstract: A comprehensive finite element method for three-dimensional simulations of stationary and transient electrochemical systems including all multi-ion transport mechanisms (convection, diffusion and migration) is presented. In addition, phenomenological electrode kinetics boundary conditions are accounted for without being limited to any specific law. The governing equations form a set of coupled nonlinear partial differential equations subject to an algebraic constraint due to the electroneutrality condition. The advantage of a convective formulation of the ion-transport equations with respect to a natural application of homogeneous flux boundary conditions is emphasized. For one of the numerical examples, an analytical solution for the coupled problem is provided, and it is demonstrated that the proposed computational approach is robust and provides accurate results.
Stichworte: finite element method, ion transport, electrolyte solution, computational electrochemistry, transient convection-diffusion-migration equation, electroneutrality condition