Finite Volume Discretization of Nonlinear Diffusion in Li-Ion Batteries

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Numerical modeling of electrochemical process in Li-Ion problems is an emerging topic of great practical interest. In this work we present a Finite Volume discretization of electrochemical diffusive processes occurring during the operation of Li-Ion batteries. The system of equations is a nonlinear, time-dependent diffusive system, coupling the Li concentration and the electric potential. The system is formulated at length-scale in which two different types of domains are distinguished, one for electrolyte and one for cathode/electrode. The domains can be of highly irregular shape, with the electrolyte occupying the pore space of a porous solid electrode. The material parameters in each domain differ by several orders of magnitude and can be nonlinear. Moreover, special interface conditions are imposed at the boundary separating the electrolyte from an electrode. The field variables are discontinuous across such an interface and the coupling is highly nonlinear, rendering direct iteration methods ineffective for such problems. We formulate a Newton iteration for the coupled system. A series of numerical examples are presented for different type of electrolyte/electrode configurations and material parameters. The convergence of the Newton method is characterized both as function of nonlinear material parameters as well as the nonlinearity in the interface conditions.