Continuum Modeling of Ca-based Batteries

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Among the various post-lithium battery materials, calcium is a promising anode material due to its high natural abundance and improved safety compared to lithium, while having only a slightly lower electrochemical potential than lithium. [1] We focus on a Ca-S cell and a battery with an anode mainly made of Ca-Sn alloys and a 1,4-polyanthraquinone cathode [2].

We model these Ca-based batteries to gain a better understanding of the processes inside the batteries. Our model considers concentrated solutions and porous electrodes. It describes the one-dimensional transport of ions from the anode to the cathode on a macroscopic scale by means of a system of differential and algebraic equations. The charge transfer reactions are modeled using Butler-Volmer kinetics. [3] We adapted this model to the battery cell with the Ca-Sn alloy anode and the 1,4-polyanthraquinone cathode [2] and parametrized it.

The difficulty in adapting the model to the Ca-S cell lies in the different sulfides which occur in the polysulfide shuttle. For each sulfide a transport equation is added, and the concentration of that sulfide or the porosity is described, respectively. [4] Compared to the Li-S cell, there are more unknows related to speciation in the electrolyte and the thermodynamics of the precipitates. We aim to parametrize the model with data from our project partners in the BMBF CaSino project.

References:
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