6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
11 - 15 June 2018, Glasgow, UK

OPTIMIZATION METHODS IN APPLICATION TO SOLID ELECTROLYTE ION TRANSPORT

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Key words: *Batteries, Solid Electrolytes, Drift-Diffusion Poisson System, Poisson-Boltzmann Equation, PDE Constrained Optimization*

Solid electrolytes (SEs) promise to be an attractive candidate for safe future battery systems due to a variety of favorable properties. However, low power densities as well as high charge transfer resistances are limiting factors of all-solid-state batteries. In this contribution mathematical modelling and simulation coupled with optimization is used to tackle the present challenges in the design of SEs. Based on the thermodynamically consistent model derived in [1], we describe the ion transport in a SE sandwiched between two blocking electrodes by a drift-diffusion Poisson system. This nonlinear partial differential equation (PDE) system allows us to determine the thermodynamic state in the SE, given by the cation concentration and the electrostatic potential, numerically. For efficient steady-state simulations, the system is reduced to a modified Poisson-Boltzmann equation. In order to find an optimal material design, methods from PDE constrained optimization are applied through the minimization of specific cost functionals according to the desired material properties. One example of the presented cost functionals is motivated by the experimental work in [2] and [3], where reduced charge-transfer resistances in dielectrically modified respectively thin film SEs where found. In sequence to our simulations we found reduced electric potential gradients in highly dielectric and thin film SEs in relation to SE thickness. Therefore, we optimize the dielectric susceptibility of our material, such that it favors an overall lower electric field. This numerical result is validated by an analytical solution.

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