Modeling of ion transport by a Maxwell-Stefan approach and numerical results

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Electro-thermodynamics provides a consistent framework to derive continuum models for the description of electrochemical systems on the device level, e.g. for batteries or fuel cells. These models must be equipped with two additional ingredients: (i) a free energy model to calculate the chemical potentials and (ii) a kinetic model for the kinetic coefficients. Suitable free energy models for liquid electrolytes incorporating ion–solvent interaction, finite ion sizes and solvation already exist and have been validated against experimental measurements.

In this work, we apply a Maxwell–Stefan setting for multicomponent transport in order to derive mobility coefficients. However, instead of these mobility coefficients, often other transport parameters are more insightful for the interpretation of measurements. In the context of energy conversion systems, the electric conductivity of electrolytes has naturally attracted most interest. Further relevant parameters are the transference numbers and diffusion coefficients. Contrary to the equilibrium properties, some of these mentioned transport properties depend on a combination of chemical potentials and kinetic coefficients, while others depend solely on the kinetic coefficients.

In a numerical study, we analyze the impact of ion solvation and incomplete salt dissociation on the transport parameters of a non-dilute electrolyte.