A Thermodynamically Consistent Continuum Model for Ion-Selective Membranes in Aqueous Batteries

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Membranes with ion-selective properties offer great potential for the improvement of novel energy storage technologies [1]. Among these technologies, aqueous batteries such as zinc-metal batteries (ZMBs) are particularly promising due to their relatively low cost, resource availability and high theoretic specific capacity [2]. For these cells, the implementation of a filtering separator is desirable, since the crossover of certain ions has been shown to contribute significantly to the degradation of the cell [3]; e.g. $Zn(OH)_4^{-2}$ in alkaline zinc-manganese oxide cells (degrading the cathode) and CO_3^{-2} in zinc-air cells (lowering the alkalinity) [4].
To gain insight for the tailored development of suitable membranes, a consistent model describing membrane transport of various species using physically meaningful parameters is required. Among the variety of available membrane models, especially the DSPM-DE model [5], the Donnan-Manning model [6, 7] and the low-T* model [8] have been proven to be applicable for some relevant membranes and certain solutes. Yet, for the intended purpose, a model with a wider applicability offering more predictive value and interpretability of the model parameters is desirable. This is achieved by combining the fundamental ideas of various models in a thermodynamically consistent manner which allows to predict qualitative trends from theory, as well as a more quantitatively accurate parameterization from experiments.
Implementation of this widely applicable membrane model into a cell scale model then allows for efficient tuning of membrane properties for the overall improvement of the battery performance.

References:
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