

MACROHOMOGENEOUS CELL MODELS FOR ORGANIC REDOX FLOW BATTERIES

The macroscale models developed at the Institute of Computational physics at ZHAW allow for the simulation of physicochemical effects within a single electrochemical cell. The continuum models describe the driving potentials and fluxes of mass and charge, the electrochemical reactions of the active material in the porous electrodes, as well as the critical transport phenomena within the membrane.



Predicted power density as a function of the state of charge (SoC) and the (discharging) electric current density using the 0D-U-I-SoC model.



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Our OD-U-I-SoC cell model predicts the cell performance with respect to the state of charge (SoC) of the battery and the electric current density. The model considers the crucial activation and concentration overpotentials at the electrode surface, as well as the electro-osmotic drag causing volume changes due to the transfer of solvent between the half-cells. The model implementation in Mathematica has been made available as open-source software on our GitHub repository.



Predicted cell voltage for a charge-discharge cycling experiment with a constant charging / discharging electric current (orange), together with experimental measurements (blue).

