

STACK AND SYSTEM MODELS FOR REDOX FLOW BATTERIES



Mathematical stack and system-level models have been developed to determine the overall system performance for different redox couples. MATLAB, COMSOL Multiphysics and high-performance computing (HPC) are used for efficient numerical modelling and simulation of the flow in the stack-manifold arrangements. The developed 3D parameterised stack geometry in COMSOL can be automatically updated with fully user-defined geometric parameters, such as the number of cells, cell size, manifold and channel sizes. Users can also vary other input parameters through an interface allowing for changes in particular chemistries with design parameters to be studied and evaluated.

While initial simulations based on the well-established vanadium redox flow battery chemistry have been used for validation, organic redox flow couples of choice can be evaluated with known properties. With the model, redox flow batteries can be simulated for their stoichiometric or applied flow rates (either constant or variable), the pressure losses of components, species concentrations, state-ofcharge, cell/stack voltages, currents (including shunt currents), resistances, energies and efficiencies. Thermal factors are also considered in the final coupled stack and system model which can be used to optimise the system efficiency of flow batteries.



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Example results:





Pressure plot for a 5-cell stack

Velocity plots with zoom-ins for a 5-cell stack



Simulation results of a charge-discharge cycle for a 40-cell stack under variable flow rates

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