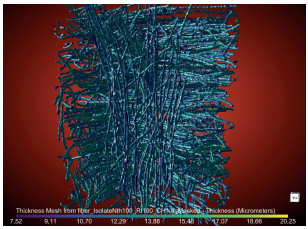
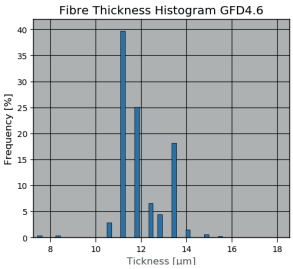
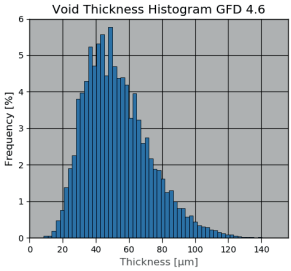
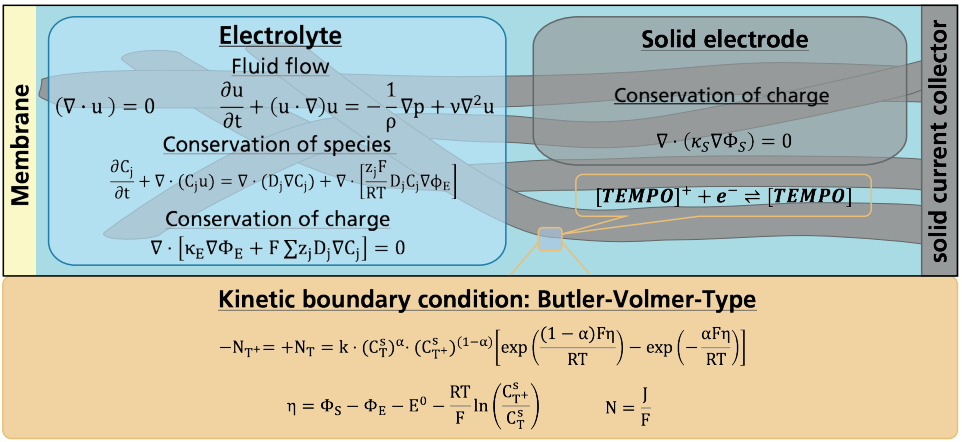
3D MICROSTRUCTURAL RESOLVED RFB CELL PERFORMANCE MODEL







Characterization and reconstruction of electrode microstructure using X-ray microtomography. Fiber and pore size distribution together with a colour-coded thickness mesh of a graphite felt.



Governing equations of the CFD half-cell model based on Finite Volume Method and with coupled fluid and solid regions. Simulation of laminar electrolyte flow and coupled charge conservation within both regions including electrochemical reaction on a digital twin of the real electrode.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement no. 875489.

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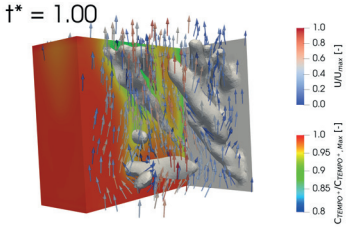
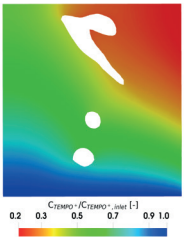
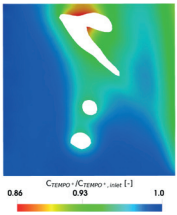


Illustration of the discharge process in the positive half-cell compartment of an organic TEMPO-based RFB system (normalized quantities). Velocity profile (arrows) of the electrolyte flow coming from the bottom to the top. Quasi steady-state TEMPO⁺ concentration profile within the electrolyte.

Three-dimensional pore-scale continuum models resolve the real geometry of the electrode to gain insight of **the microstructural processes inside the flow battery.** They offer great capability to obtain information about the microstructure and how it **affects transport processes** within the electrode and the overall **cell performance.**





Most of the flow battery modelling approaches to date have concentrated on volume-averaged or macroscopic calculation of transport processes within porous electrodes captured by using empirical relations e.g. Darcy's law or Bruggeman correction. Hence, the behaviour of key parameters like ionic diffusivity or permeability on performance is not represented correctly, as well as the coupled species and charge transport. Pore-scale resolved models overcome these disadvantages and provide **spatial characteristics of velocity, concentration or current density** depending on the complex structures of the electrode. Therefore, a spatially resolved continuum model is set up to gain insight into the micro-structural processes inside the flow battery.

The three-dimensional half-cell model is parameterized with the known model chemistry of the organic **4-OH-TEMPO** system and accounts for electrolyte flow, mass and charge transport. The electrochemical reaction is implemented using **Butler-Volmer type kinetics** to couple the solid and electrolyte region. The simulations consider galvanostatic and isothermal operating conditions comprising laminar and steady-state flow.

Simplified structured electrodes are used as computational domain to numerically investigate the influence of the initial active material concentration, the current density and the active surface. Furthermore, a **digital twin** of the real electrode microstructure is generated by experimental image reconstruction **from X-ray computed micro-tomography** and used to investigate the impact of different flow rates on the concentration distribution within the electrolyte and on the half-cell potential.

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