Research group Membrane Materials and Processes

Optimizing the 3D Microstructure of Redox Flow Battery Electrodes

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Need for large-scale energy storage

Integrating renewable energy technologies into the grid is necessary to enable a sustainable energy economy. However, their intrinsic intermittency (Figure 1) motivates the development of low-cost, large-scale energy storage systems, in the pursuit of filling the gap between renewable energy generation and consumers demands.

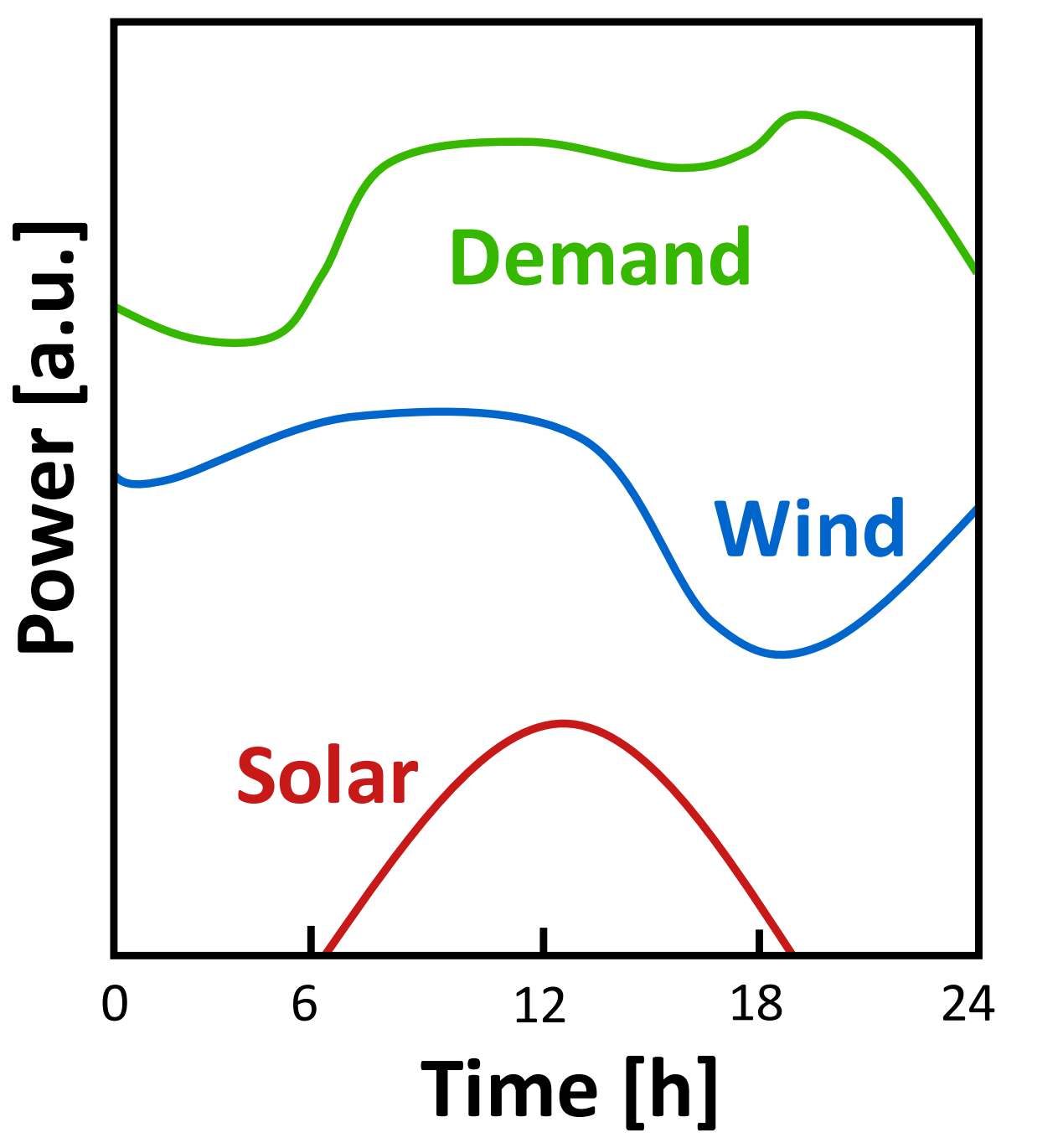


Figure 1: Mismatch between renewable energy generation and demand in Germany (02/2018).[1]

Redox Flow Batteries (RFBs)

Redox flow batteries (RFBs) (Figure 2) are rechargeable electrochemical reactors that are promising for grid storage due to the possibility to decouple energy (i.e. tank volume) and power (i.e. reactor size), facilitating their large-scale deployment[2]. Porous electrodes need to fulfil several performance-relevant functions which impact the overall efficiency creating the possibility to reduce the costs of the RFB.

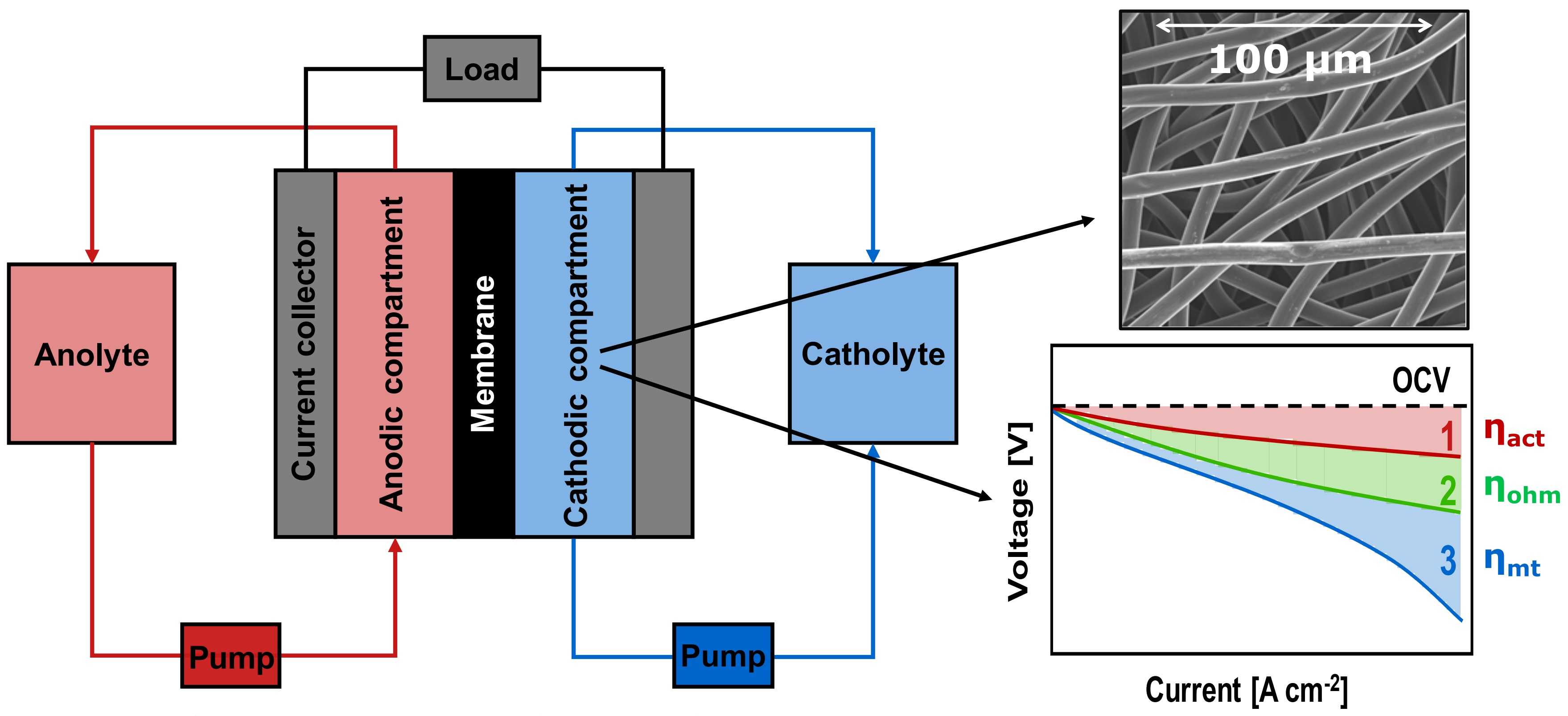
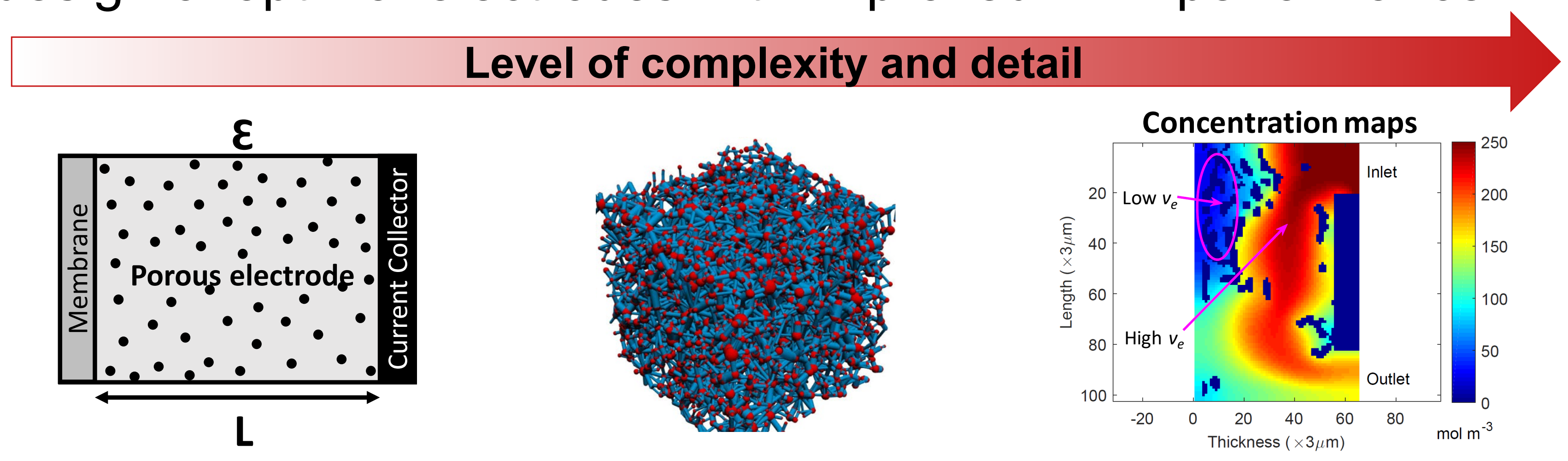


Figure 2: Schematic diagram of a redox flow battery, the porous electrode and the discharge polarization curve showing the three main losses: mass transfer, ohmic and activation losses.

Computer aided-design

Multiphysics simulations are used to understand the influence of the electrode microstructure with increasing level of detail (Figure 3). These learnings are leveraged for the bottom-up design of optimal electrodes with improved RFB performance.



1D - Macrohomogenous **3D** - Pore Network Model[3] **3D** - Lattice Boltzmann[4] or Finite element method

Figure 3: Overview of various multiphysics simulations with increasing complexity.

Network extraction

Using X-ray tomography and the SNOW algorithm[3], a pore network can be extracted from an electrode (Figure 4), which can be validated and used in a pore network model (PNM).

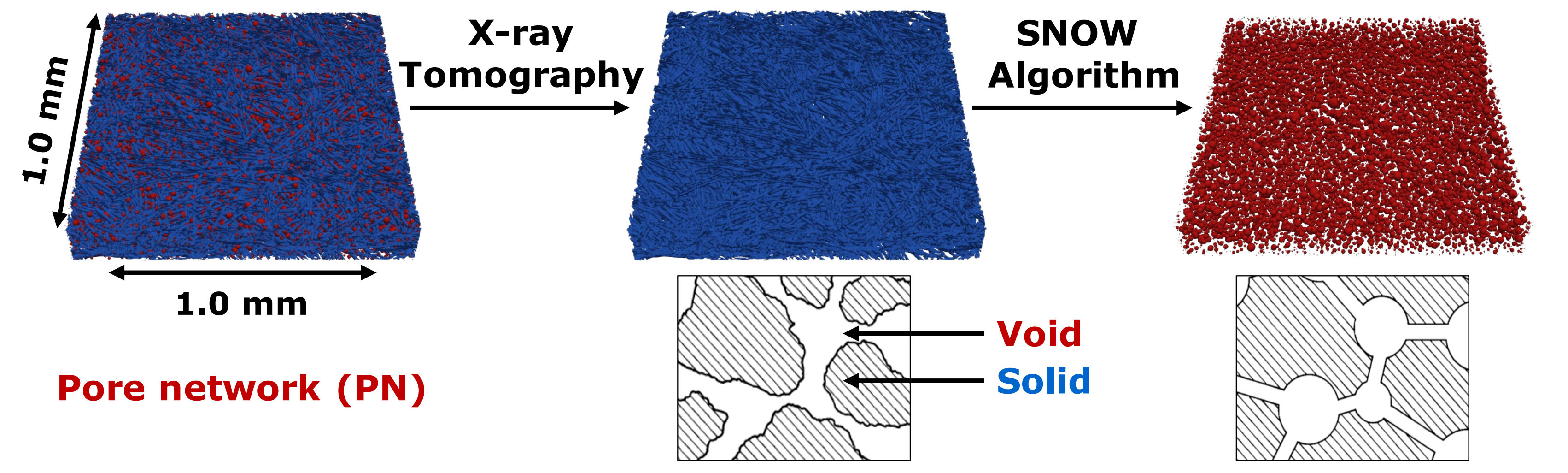


Figure 4: Visualization of an extracted pore network for a Freudenberg electrode.

Pore network model (PNM) validation

We developed a three-dimensional, electrochemical modelling toolkit integrated in an open access platform (OpenPNM[5]). The simulation domain is electrolyte-agnostic and computes the electrolyte fluid transport (1), species transport (2) and charge transport (3) (Figure 5) at low computational cost.

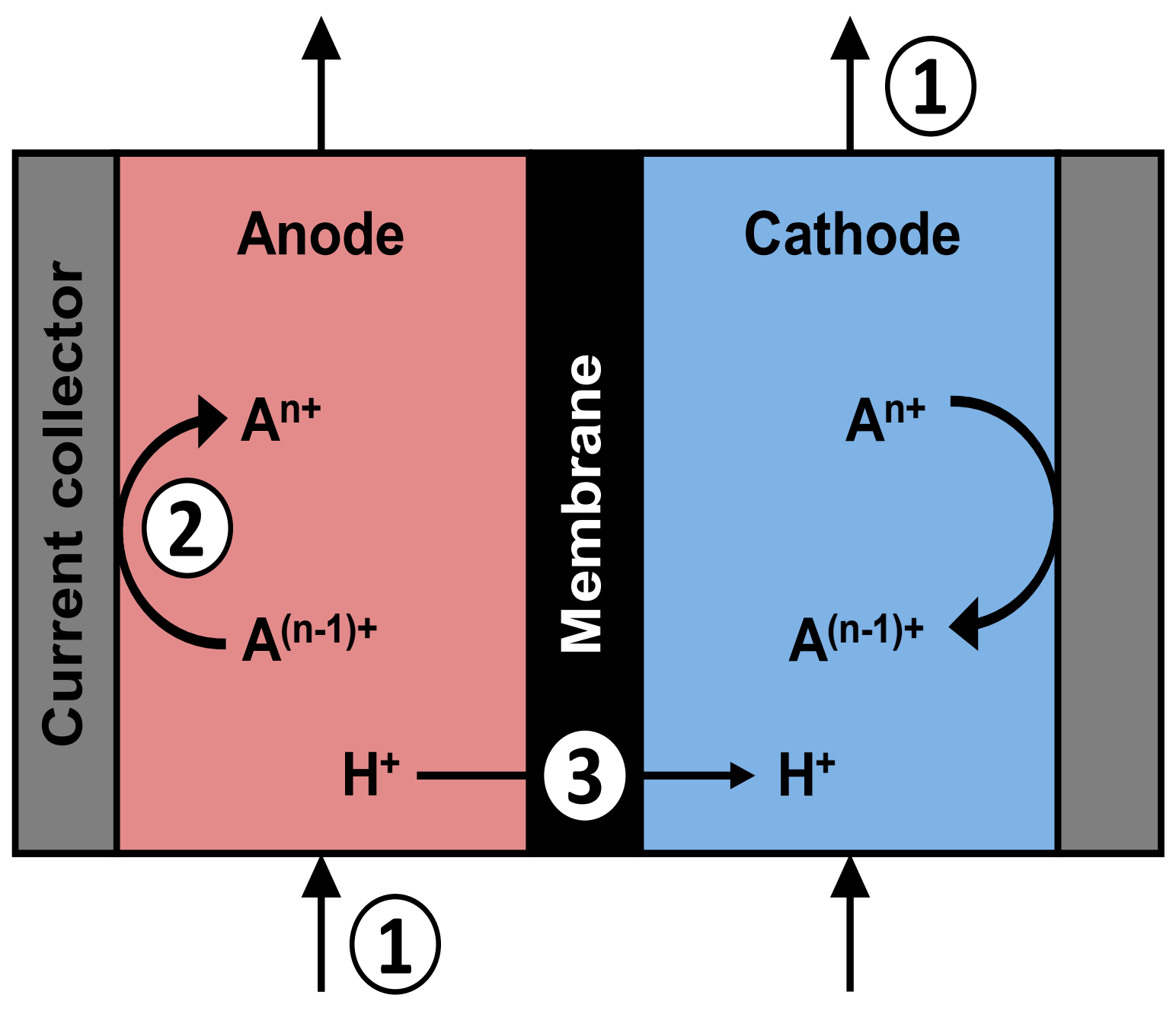


Figure 5: Schematic representation of the PNM domain.

The PNM was validated using a symmetric cell (Figure 6):

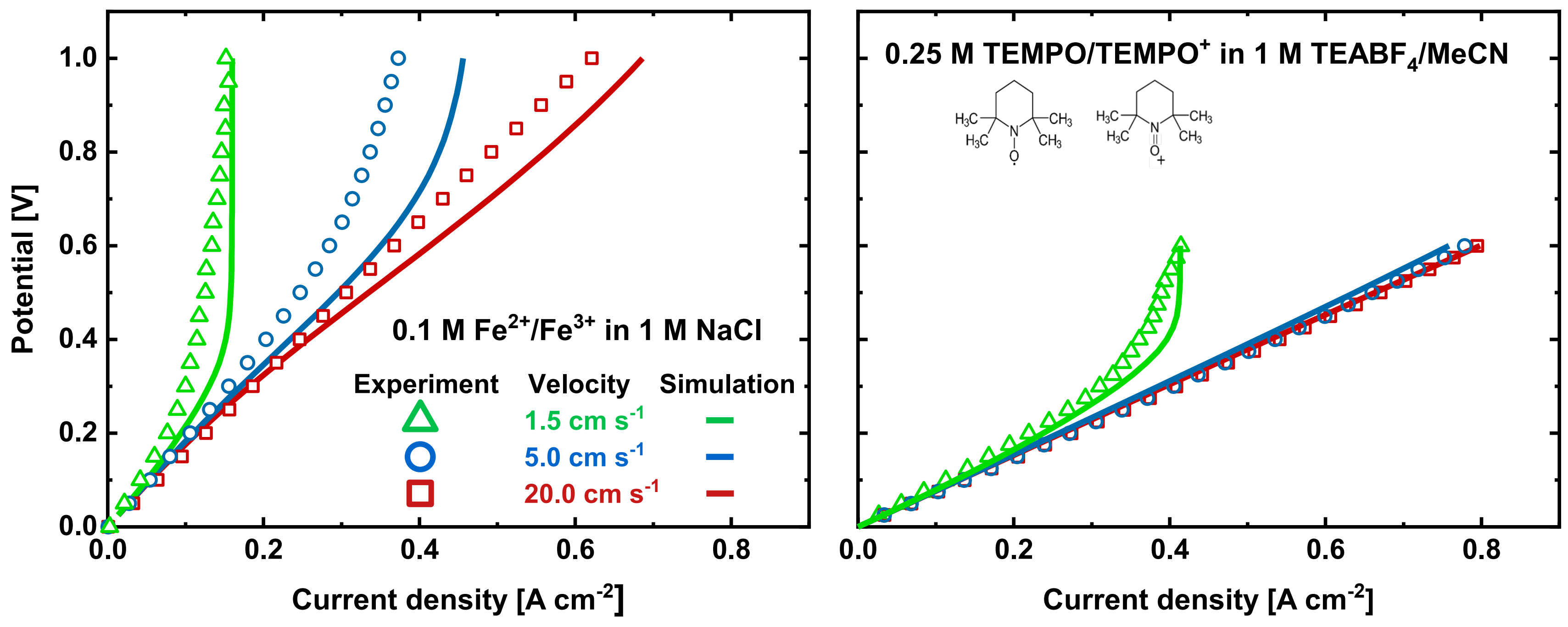


Figure 6: Cell potential at 20, 5, and 1.5 cm s^{-1} electrolyte velocity for the Freudenberg electrode. A single electrolyte cell with an organic (TEMPO/TEMPO$^+$) and inorganic electrolyte (Fe^{2+}/Fe^{3+}) was used.

Acknowledgements

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References

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