Multi-{physics, phase, scale} computational modeling of interface-coupled problems in redox flow batteries

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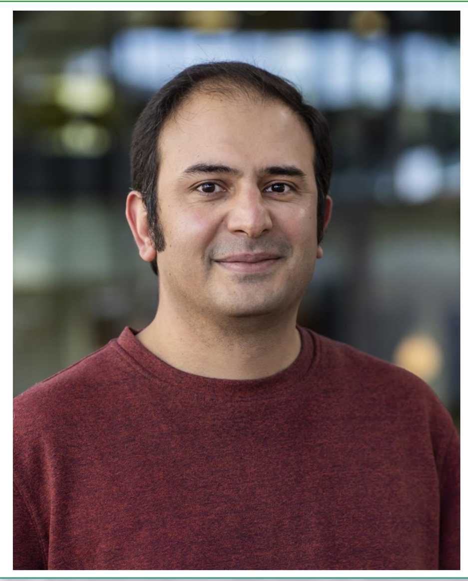

Background

- Redox flow batteries (RFBs) are gaining prominent attention for addressing the urgent need of deploying large-scale energy storage technologies to integrate intermittent renewables.
- RFBs have interesting features including higher durability and power-energy decoupling.
- Large-scale deployment of RFBs has feasibility issues regarding costs and efficiency.
- Coupled multi-scale computational models can accelerate our understanding of intricate RFB processes, providing a unique perspective to guide the design of RFB components.

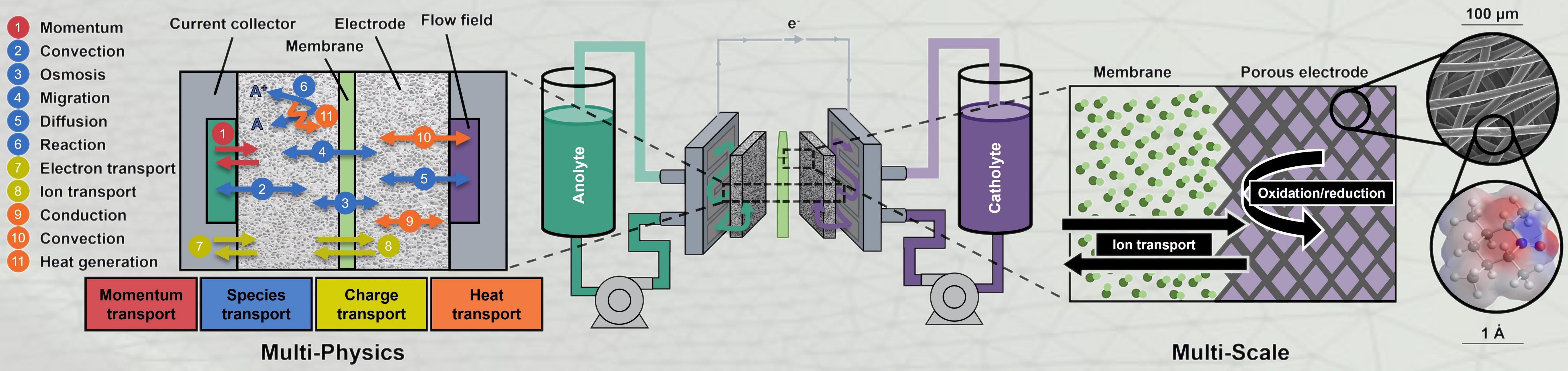

Fig 1: In RFBs, electrolyte solution containing dissolved or suspended active species is stored in external tanks and pumped through the electrochemical stack where the active species undergo electrochemical reactions to charge/discharge the battery.

Methodology

- In this research, we are developing multi-{physics, phase, scale} models of the RFB processes.
- These processes range from transport phenomena on the cell level to the microstructure effects on the pore-scale.
  - **Macro-scale**: Finite element/volume methods to solve electrochemical reactions equations.
  - **Meso-scale**: Lattice Boltzmann method (LBM) for the flow through the porous electrode.
  - **Nano-scale**: Density functional theory (DFT) to model the kinetic rates of reactants.

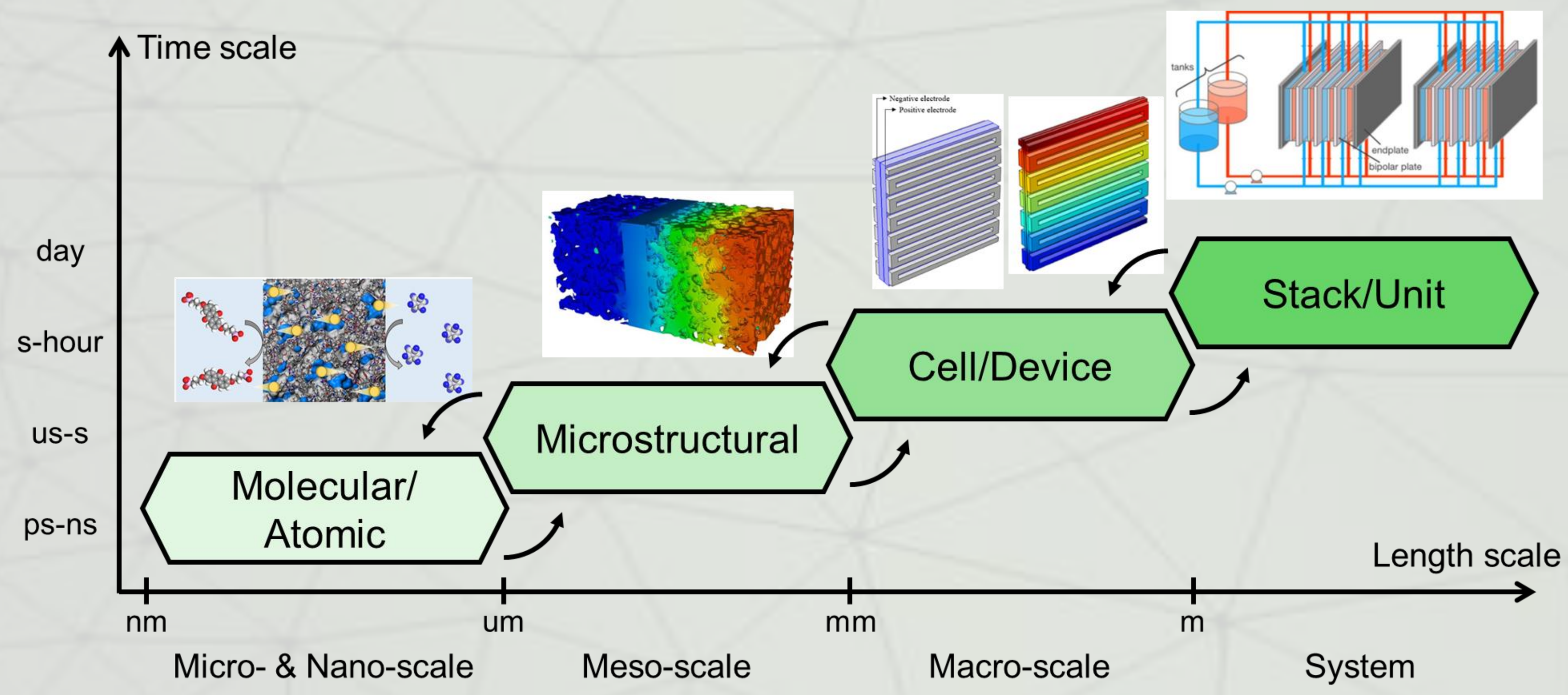

Fig 2: Various time and length scales in RFBs (figures adapted from [1-4]).

Meso-scale

- Pore-scale simulations are essential to understand how pore shape and transport impact the RFB performance.
- LBM excels in handling complex multi-phase phenomena and high-performance computing, making it suitable for pore-scale simulations when a high resolution is required.

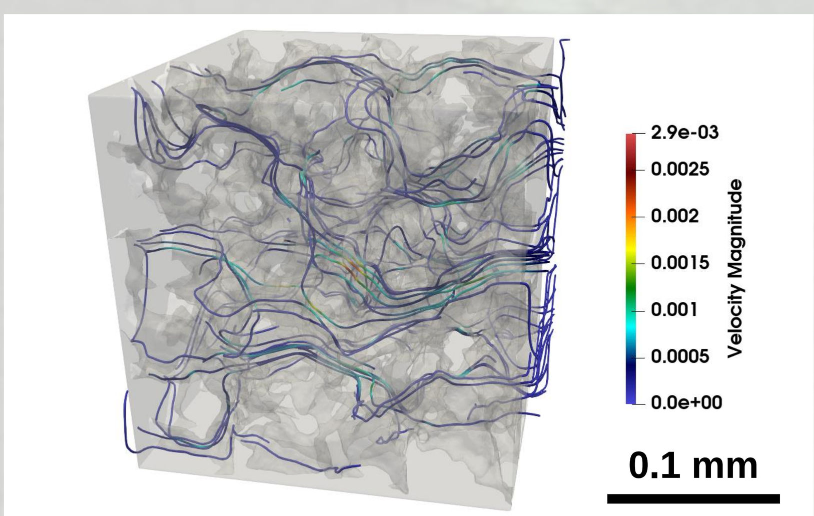

Fig 3: Single-phase simulation of flow inside a porous electrode. Colors show the magnitude of the velocity field plotted over the streamlines.

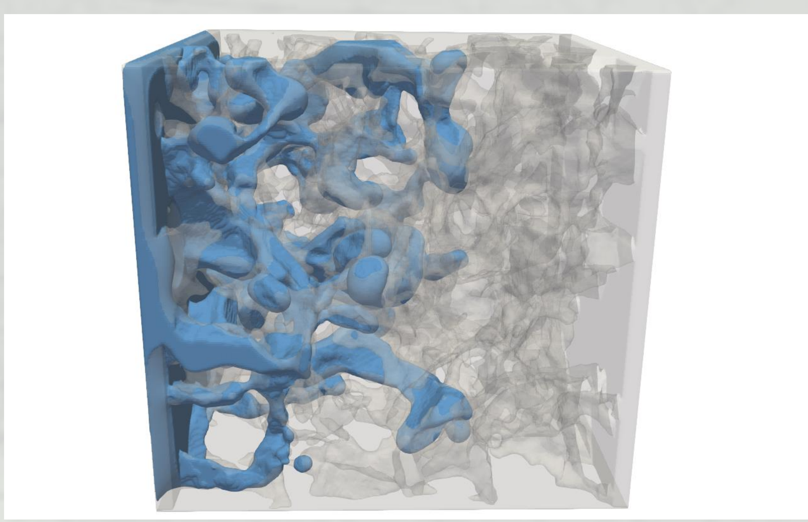

Fig 4: Multi-phase simulation of flow inside a porous electrode, where first phase (plotted in blue) removes and replaces the second phase (not plotted).

Macro-scale

- Macro-scale transport equations provide insights into how reactor design influences RFB performance, which can be simulated by high-performance numerical methods applied to the entire reactor setup's computational mesh.

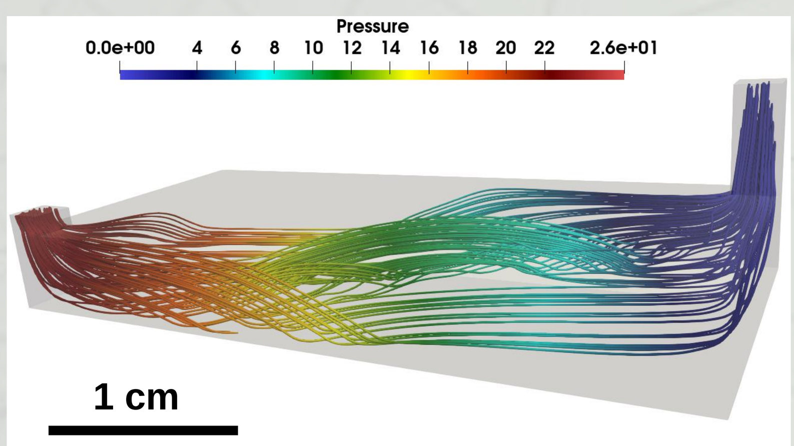

Fig 5: Flow simulation inside a porous electrode represented as a solid block with variable porosity (inlet on the left and outlet on the right). Colors demonstrate the reference pressure drop plotted over the streamlines of the velocity field.

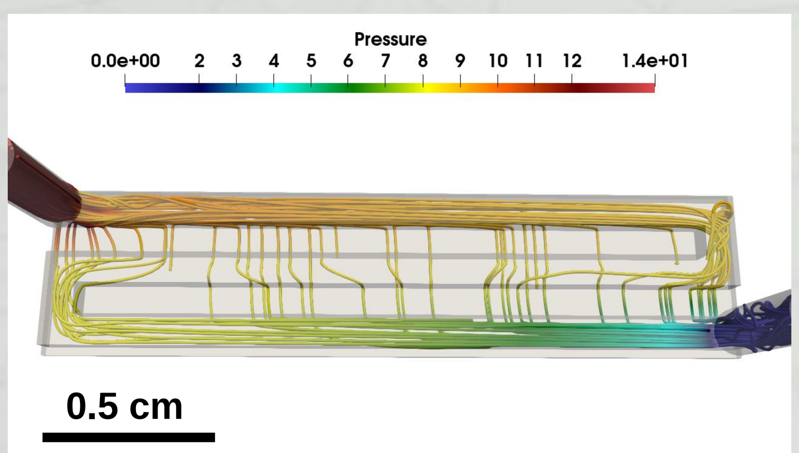

Fig 6: Flow simulation inside a half-cell setup of an RFB, in which the flow field (fluid channel) is positioned on top a porous electrode modeled by Darcy equation. Colors show the reference pressure drop plotted over the streamlines.

Acknowledgements

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References

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