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

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ABSTRACT

Motivated by an urgent need to deploy large-scale energy storage technologies to integrate intermittent renewables, redox flow batteries (RFBs) are gaining prominent attention due to their interesting features including higher durability and power-energy decoupling. RFBs are rechargeable electrochemical systems in which an electrolyte solution containing dissolved or suspended active species is stored in external tanks and pumped through the electrochemical stack - consisting of flow fields, porous electrodes, and membranes - where the active species undergo electrochemical reactions to charge/discharge the battery. However, large-scale deployment of RFBs has feasibility issues regarding costs and efficiency, which can be tackled by tuning their multi-scale design parameters [1].

Developing a coupled multi-scale computational model for RFBs can facilitate our understanding of the interplay between intricate phenomena occurring at several length and time scales (depicted schematically in the figure), ranging from transport phenomena, i.e., mass, charge, momentum, and heat, on the cell level (macro and meso scales) to microstructure effects and wettability behavior on the pore-scale (micro and nano scales). Furthermore, the modeling framework should capture the reaction kinetics and multi-phase chemistry of emerging flow battery concepts (e.g. metal-air) including plating and stripping reactions [2].

In this research, we are developing a multi-{physics, phase, scale} model for the optimization of next-generation RFBs in the cell-, electrode-, and pore-scale. The model includes free fluid flow (representing flow field channels) over a porous medium (porous electrode) and solves the transport mechanisms over the entire computational domain with a focus on the electrolyte-electrode interface. The model is developed using finite element/volume methods combined with pore network modeling techniques, implemented using various open-source modeling frameworks including OpenFOAM [3], FEniCS [4], and OpenPNM [5].

In this presentation, I will first discuss the structure of the modeling framework including the continuum transport models, the pore network model, and the employed numerical schemes. Then, I will present the coupling between continuum and porous medium models. Finally, I will highlight some initial results focused on the efficiency of the coupling of the electrolyte fluid transport with the porous medium and pore network representation of the electrode [6]. We hope that the developed model can be a functional tool to assess and optimize RFB materials and operating conditions and can be broadly adopted to model emerging flow battery chemistries.

References

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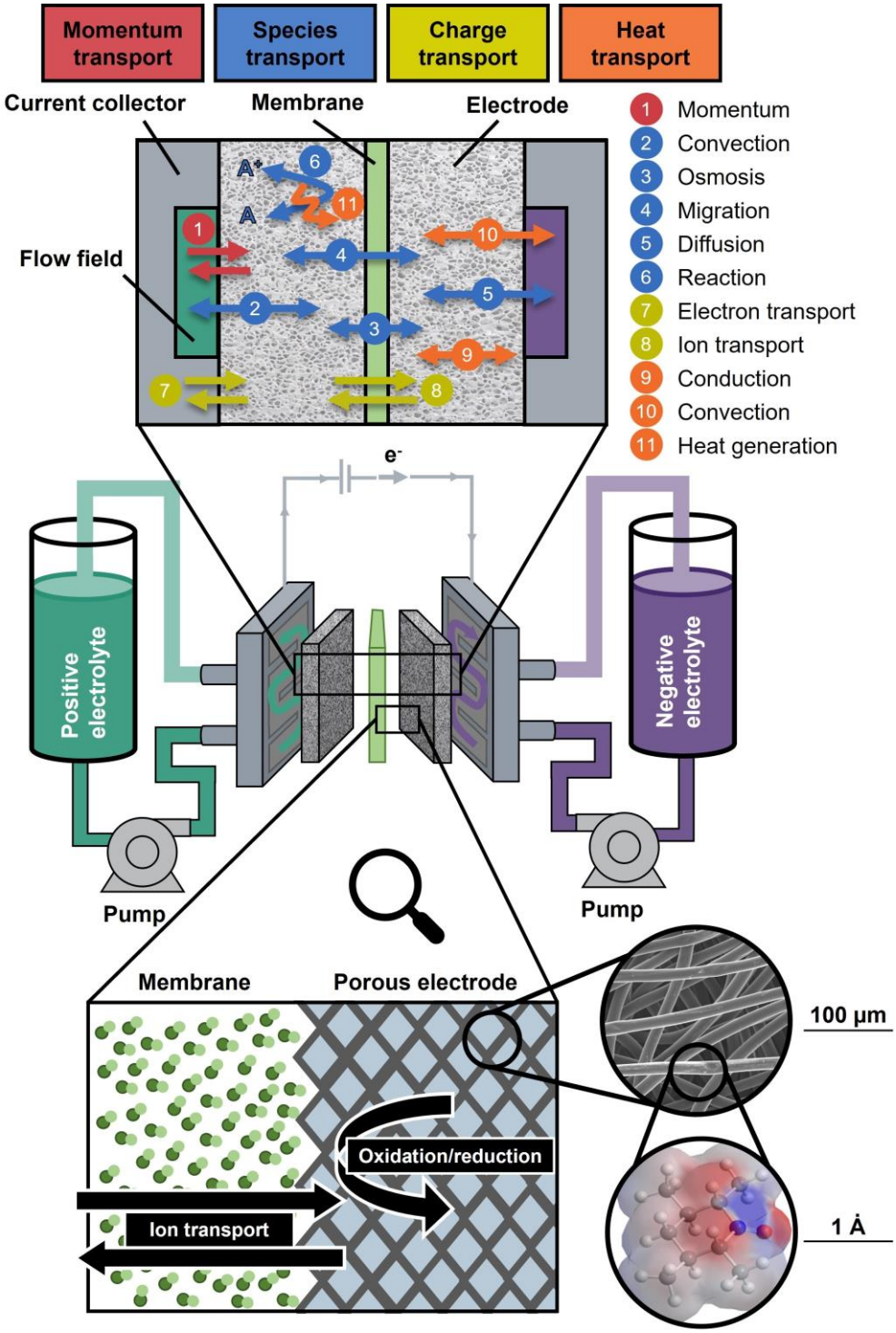

Figure 1: Schematic representation of the structure of a redox flow battery as well as a summary of the transport phenomena occurring on the cell level (top) and a zoomed view on the porous electrode depicting the multi-scale nature of these phenomena on the pore-scale (bottom).