Contribution ID: **85** Type: **Oral Presentation**

How to design a 3D ordered microstructure for redox flow batteries: A pore network modeling study

Tuesday, 31 May 2022 15:05 (15 minutes)

Amid growing energy demand and the progressive contribution of intermittent renewable energy, the need for large-scale energy storage systems have become critical. Redox flow batteries can be a legitimate choice to store a huge amount of energy, subject to further improvement in their components, specifically the porous electrode. 3D printing technology is a viable method to manufacture porous electrodes with an engineered design and controllable properties. Attaining this goal requires an understanding of the effect of electrode microstructure which this study strove to provide. The effect of different parameters, including pore size, throat size, frequency of lattice units, and permeability anisotropy in the through-plane and in-plane directions were investigated in the flow-through as well as interdigitated batteries.

Pore network modeling was utilized to investigate the effect of microstructure on the performance of Hydrogen-Bromine (H2-Br2) flow batteries. Simulations were carried out under steady-state conditions for electrolyte transport, species transport, and charge transport. To isolate the role of microstructure on the performance of the battery, simulations were performed at the constant flow condition in which the advective force was constant.

The simulations were validated against the experimental study using an unstructured pore network, extracted from a tomography scan of a commercial carbon paper. A 3D printed ordered cubic lattice with the same permeability of the carbon paper showed a better performance. This was mainly achieved by better mass transport as a result of higher advection, diffusion, and lower tortuosity of the ordered lattice.

It was found that a combination of bigger pores and smaller throats at constant permeability, facilitated the diffusion rate especially in the in-plane direction, as well as, increased the specific surface area of the network. It was also shown that a larger number of lattice units, resulted in a higher surface area, consequently a higher current generation.

For both of the flow-through and interdigitated flow fields, permeability change in the through-plane direction (x-direction and y-direction) at the constant flow rate condition, almost did not affect the performance of the battery. However, the latter drastically changed the required electrolyte supplying pressure that could translate into a more economically feasible process. The permeability variation in in-plane direction reinforced or hampered the diffusion and also the current generation.

Finally, an improved design of microstructure for the flow-through and interdigitated batteries were proposed and investigated. The specific surface area, permeability, and flow rate were kept constant to solely observe the role of microstructure on the battery performance. Results presented the superior performance of the improved microstructure in both flow fields. It was achieved by deviating the electrolyte main flow path, to the proximity of the membrane, where more reactions were taking place. This study took an initial step and provided insight into designing and manufacturing a porous electrode using 3D printing technologies. However, it can be continued in various paths including using complex 3D pore structures rather than simple cylindrical lattice to optimize the hydrodynamic behavior of the electrolyte and the specific surface area of the electrode.

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Participation

Online

Primary author: Mr SHOKRI, Javad (University of Manchester)

Co-authors: Dr BABAEI, Masoud (University of Manchester); NIASAR, Vahid (University of Manchester)

Presenter: Mr SHOKRI, Javad (University of Manchester)

Session Classification: MS22

Track Classification: (MS22) Manufactured Porous Materials for Industrial Applications