Contribution ID: **153** Type: **Oral Presentation**

Redox Flow Battery operation may be limited by "Hot Spots"observed in pore scale simulation of flow in carbon fibre felt electrodes

Friday, 4 June 2021 11:10 (15 minutes)

The Vanadium Redox Flow Battery (VRFB) is one of the most promising Electro-Chemical Device (ECD) technologies for large scale local storage of renewable energy, such as wind and solar. Commercial exploitation of this technology has emerged, but a lack of fundamental understanding regarding VRFB operation is limiting the development of this new technology. In particular, the energy density must be improved. For this reason, we investigate here the performance of carbon fibre electrode materials using a combination of computational modelling and experimental characterisation. In particular, the surface area of the porous electrode is critical to the device performance. To optimize electrochemical reactions in the electrode, the reactive surface area has to be as large as possible. In terms of micro-structure, this means that the felt fibres must be distributed homogeneously. In current VRFB technology, however, the felts are woven bundles of fibres yielding a large local variation in voids and bundles. Recently, synchrotron micro-CT scanning was used [1] to image the 3D pore structure of a graphite felt in-operando. However, the resulting alteration of the flow field could not be quantified, as it is difficult to measure in-situ due to limited spatio-temporal resolution. Also, it is difficult to obtain the altered flow field from average tortuosity and porosity calculations, as the relation between permeability and tortuosity / porosity is only known empirically. Here we calculate the relation between flow and altered micro-structural properties using direct flow calculations in pore space images of a representative volume of a carbon fibre material obtained from micro-CT imaging. We consider a 3D fibre felt geometry, obtained from micro-CT experiments, and the corresponding flow field, as a test for large volume calculations. The flow field was calculated using our home-grown Lattice-Boltzmann (LB) code (see [4]) on a big data set of 15 billion voxels using HPC facilities. we observe that the electrolyte is concentrated in local areas ("hot spots"), thus limiting electrochemical reactions. The heterogeneity of the commercial soft carbon fibre material may reduce the efficiency of the electrode, due to high voltage spots and damage in the electrode. In addition, under certain electro-chemical conditions, H2 and O2 gas bubbles may develop in the pore space of the heterogeneous electrode, which has a detrimental effect on VRFB performance [1]. Therefore we extend our multi-phase LB code to investigate the development of gas bubbles in the electrode (Fig.1b), initially by seeding random gas bubbles, based on our previous work on multi-phase flow in natural porous materials [2,3]. To mitigate problems associated with the heterogeneous nature of carbon fibre graphite felts, we propose a rational design approach to develop new carbon materials with superior properties.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

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[3] Zacharoudiou, I., Chapman, E., Boek, E.S. & Crawshaw, J. (2017) "Pore-filling events in single junction micro-models with corresponding lattice Boltzmann simulations", Journal of Fluid Mechanics, 824, 550-573. doi:10.1017/jfm.2017.363
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Session Classification: MS22

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