SEMS: RESEARCH PROJECT DESCRIPTION

1. Project Background and Description

Rational design of novel materials for flow battery and fuel cell applications

Here we propose the rational design of new materials for Electro-Chemical Devices (ECD), including the Vanadium Redox Flow Battery (VRFB) and hydrogen fuel cell (HFC).

The VRFB is one of the most promising ECD technologies for large scale local storage of renewable energy, such as wind and solar. A lack of fundamental understanding of VRFB operation, however, is limiting the development of this new technology. In particular, battery longevity is a problem due to degradation of the graphite felt carbon fibre electrode material under electrochemical cycling. In addition, the energy density must be improved, as this is low compared to Li-ion battery performance. For these reasons, we propose here to investigate the performance of novel electrode materials in comparison with industry-standard graphite felt carbon fibre electrodes using computational modelling in comparison with experimental characterisation. 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. In addition, it is very difficult to quantify the alteration of the micro-structure and flow field of the electrode using experimental techniques such as micro-CT. Here we propose to quantify the relation between flow and altered micro-structural properties using direct flow calculations in pore space images of fibres obtained from micro-CT imaging. As a preliminary result, we show in Figure 1 a representative 3D fibre geometry, obtained from micro-CT experiments, and the corresponding flow field. The flow field was calculated using our home-grown Lattice-Boltzmann (LB) CFD code (see [1], [2] and [3]) on a big data set of 15 billion voxels using HPC facilities.

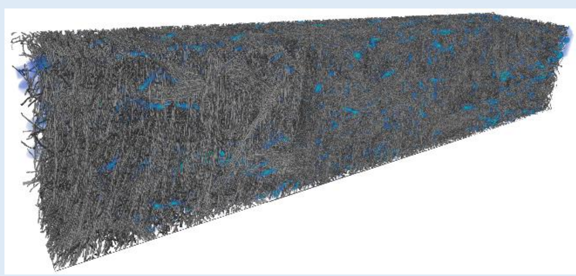

Figure 1: Micro-CT pore space image of carbon fibre felt combined with LB calculations of the flow field. Blue colour indicates “hot spots” in the flow field.

From this figure, we observe that the electrolyte is concentrated in local areas, thus limiting electro-chemical reactions. The heterogeneity of the carbon fibre material reduces the efficiency of the electrode, as it may cause high voltage spots and therefore damage in the electrode. To quantify this observation, we propose to further develop our LB code to include reactive transport in electrode materials in the carbon fibre pore space, based on my previous work [3]. In addition, under certain electro-chemical conditions, H_2 and O_2 gas bubbles develop in the pore space of the heterogeneous electrode, which has a detrimental effect on VRFB performance. To mitigate this, we propose to extend our LB code to multi-phase gas-liquid flow, based on my previous work [1,2]. Modelling results will be validated against experimental results using in-situ micro-CT flow cells. To mitigate problems associated with commercial carbon fibre graphite felts, we propose a rational design approach to develop new carbon materials with superior properties. For this purpose, we will use neural networks and try to extend the Generative Adversarial Network (GAN) approach proposed by Cooper *et al*. [4] in comparison with Normalising Flow (Greg Slabaugh, QMUL) as an alternative to GANs as an emerging topic [5].

This project will be carried out in collaboration with co-supervisor Dr Ana Sobrido at QMUL, who just secured a £1.4m UKRI Future Leaders Fellowship (FLF) award to develop next-generation flow batteries capable of storing large amounts of excess energy from sustainable sources, helping to move the UK away from fossil fuels.

[1] Zacharoudiou, I., Chapman, E., Boek, E., & Crawshaw, J. (2017), Journal of Fluid Mechanics, 824, 550-573. doi:10.1017/jfm.2017.363

[2] Zacharoudiou, I., Boek, E.S., & Crawshaw, J. (2018), Nature Scientific Reports, 8:15561 DOI:10.1038/s41598-018-33502-y

[3] F.Gray, S. Shah, J.Crawshaw, B.Anabaraonye, E.S. Boek (2018), Advances in Water Resources. 121, 369-387.

[4] Gayon-Lombardo, A., Mosser, L., Brandon, N.P. et al. Pores for thought: generative adversarial networks for stochastic reconstruction of 3D multi-phase electrode microstructures with periodic boundaries. npj Comput Mater 6, 82 (2020). (https://doi.org/10.1038/s41524-020-0340-7)

[5] https://medium.com/swlh/why-i-stopped-using-gan-eccv2020-d2b20dcfe1d

2. Project Scope

Three research project objectives

1) Develop computational methods for reactive / multi-phase flow at the pore scale in electrochemical devices.
2) Use experimental imaging techniques including micro-CT and FIB-SEM to acquire pore scale images
3) Develop a rational design approach to identify novel and superior electrode / catalyst support materials

3. Desired Skills from the Student

Key skills needed for the PhD project

1) Undergraduate degree in science or engineering
2) Interest in computational methods and developing code
3) Interest in using experimental imaging techniques including micro-CT and FIB-SEM

4. Supervisory Team

Add supervisory team details

Primary supervisor: Dr Edo Boek, SEMS, e.boek@qmul@ac.uk

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