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Pore-scale study to understand the influence of porosity on mass transport in Anodic Porous Transport Layer of PEM electrolyser using Lattice Boltzmann Method

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The surging demand for energy and the environmental impacts of conventional sources such as fossil fuels are the ground for the upcoming predicted energy crisis. Electrolysis of water has emerged as a promising technology for surplus production and storage of pure hydrogen as an alternative green fuel. Polymer Electrolyte Membrane (PEM) water electrolyzers are used for the on-demand power generation without any greenhouse gas emissions. The anodic Porous Transport Layer (PTL) of PEM electrolyzers serves channels for water to reach the active sites of the catalyst layer as well as escape pathways for oxygen. The material properties of the anodic PTL such as porosity, pore size distribution, fibre thickness and tortuosity play a major role in the performance of the PEM electrolyzers. Anodic PTL has a fibrous porous structure in which pore volume is larger than the throat volume. This results in oxygen bubble snap-off and fast finger generation according to the local porosity variation in the PTL which ultimately affects the efficiency of the oxygen removal process. However, this cannot be studied using well-established Pore Network Modelling (PNM) as in the reconstruction step, the pore volume is regarded as smaller than the pore volume. On the other hand, mesoscale models such as Lattice Boltzmann Model (LBM) [1] has emerged as a promising technique for simulating such fluid transport and flows in porous media [2]. In this study, a multicomponent Shan Chen LBM is implemented to study the evolution of oxygen-water phase distribution in 3D anodic PTL of the electrolyser. The PTL features such as porosity and pore size distribution are studied for the minimization of oxygen saturation. The porosity of the PTL can be varied by the thickness of the fibres and the number of the fibres. The influence of these two parameters at the same porosity of the PTL is studied in detail which further affects the performance of the electrolyser. Moreover, bubble snap-off, bubble coalescence, and slug flow of oxygen finger are discussed in a three-dimensional fibrous anodic PTL. This work is a fundamental step to understand the morphology of the anodic PTL to enhance the rate of oxygen removal by rapid bubble coalesce and water delivery to the active sites of the catalyst layer.

Time Block Preference

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

References

- [1] A.K. Gunstensen, D.H. Rothman, S. Zaleski, G. Zanetti, Lattice Boltzmann model of immiscible fluids, *Phys. Rev. A.* 43 (1991) 4320–4327. doi:10.1103/PhysRevA.43.4320.
- [2] D. Panda, S. Bhaskaran, S. Paliwal, A. Kharaghani, E. Tsotsas, V.K. Surasani, Pore-scale physics of drying porous media revealed by Lattice Boltzmann simulations, *Dry. Technol.* (2020).

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