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Lattice Boltzmann simulations of invasion in porous transport layer (PTL) at anode side of polymer electrolyte membrane (PEM) water electrolyser

Tuesday, 1 June 2021 19:00 (1 hour)

Among the demanding challenges of the 21st century, clean energy supply is still challenging to the scientific community to mitigate global warming. In this regard, transforming renewable energy into a stable and reliable fuel form by electrochemical methods is a promising technology. The polymer electrolyte membrane (PEM) water electrolysis is a key technology which uses water as feedstock for hydrogen production. The efficiency of PEM electrolysers is mainly due to well-coupled kinetics of flow and reaction that occur inside the porous electrodes. The microstructure inside the anodic PTL plays a major role for favourable kinetics by facilitating counter-current transport of water and oxygen. In this study, we elucidate the transport mechanisms inside the PTL for invasion of oxygen using Lattice Boltzmann method (LBM). A multiphase and multicomponent LBM (Shan Chen LBM) [1] is applied based on BGK collision operator. LBM simulations are used in optimising the structural parameters of PTL (i.e. pore structure, pore connectivity, pore shape) for efficient operation of water electrolyser. As a first step, LBM simulation for titanium felt PTL is compared with experimental data from literature as well as pore network modelling (PNM), see Figure 1. The Capillary number (Ca) and Bond number (Bo) are used to study the competitiveness between the capillary and viscous forces and gravity for understanding the evolution of invasion patterns. Further, LBM simulations for imbibition and drainage phenomena inside the anodic PTL will be shown and discussed based on a titanium felt PTL.

Figure 1: LB simulation invasion patterns for titanium felt PTL, comparison with experimental results from literature [2] and PNM simulations [3].

Time Block Preference

Time Block C (18:00-21:00 CET)

References

[1] G. T. Zachariah, D. Panda, and V. K. Surasani, “Lattice Boltzmann simulations for invasion patterns during drying of capillary porous media,”Chem. Eng. Sci., 2018, doi: 10.1016/j.ces.2018.11.003.
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[3] H. Altaf, N. Vorhauer, E. Tsotsas, and T. Vidaković-Koch, “Steady-state water drainage by oxygen in anodic porous transport layer of electrolyzers: A 2D pore network study,”Processes, vol. 8, no. 3, 2020, doi: 10.3390/PR8030362.

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