Optimizing Porous Transport Layer through Lattice Boltzmann Simulation

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Highlights

- Water needs to overcomes backpressure to reach catalyst layer.
- Two novel PTL structures were proposed to eliminate negative pressure gradients.
- Oxygen removal rate increases approximately tenfold with our PTLs.

1. Introduction

Hydrogen's high calorific value, carbon-free nature, and storage capabilities make it versatile across industries. Water electrolysis, particularly when powered by renewable energy, is widely considered the future of hydrogen production [1]. Among various electrolysers, the Proton Exchange Membrane (PEM) Water Electrolyser is favored over alkaline water and solid oxide electrolysers due to its higher working current density, overall efficiency, hydrogen gas concentration, gas pressure, and dynamic response speed. The anode porous transport layer (PTL) facilitates water access to the active sites of the anode catalyst layer (CL) and provides pathways for O_2 escape. However, high current densities lead to increased H_2 and O_2 production, resulting in a reduction of available active sites at the CL due to elevated O_2 production. Trapped O_2 bubbles impede water movement to the CL, hindering H_2 production. Therefore, optimizing the PTL structure to enhance gas removal holds promise for improving the efficiency of the PEM water electrolyser. This study aims to enhance gas removal efficiency by optimizing the anode PTL structure. The Immersed Boundary Method - Phase Field Model - Lattice Boltzmann Method (IBM-PFM-LBM), a method previously developed by our team [2], was utilized. Through simulations, two PTL designs were devised: the straight through-hole PTL with baffles and the Tesla through-hole PTL with baffles, with the objective of enhancing gas removal.

2. Methods

The removal of oxygen in the anode PTL is a complex process influenced by various factors, including the interaction between gas and liquid in a two-phase flow, fluid-wall interactions, and the hydrophilic properties of the PTL. To investigate oxygen removal from the anode PTL, we utilized a lattice Boltzmann simulation, integrating the Immersed Boundary Method (IBM) and Phase Field Model (PFM), as illustrated in Table 1.

Table 1. Equations of IBM-PFM-LBM

Governing equations of fluid		
$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho \boldsymbol{u})=0$	Continuum equations	Eq. (1)
$\frac{\partial \rho \boldsymbol{u}}{\partial t}+\nabla\cdot(\rho \boldsymbol{u}\boldsymbol{u})=\nabla\cdot\left[\rho\nu\left(\nabla\boldsymbol{u}+\nabla^T\boldsymbol{u}\right)\right]-\nabla\cdot\boldsymbol{P}+\boldsymbol{F}_b+\boldsymbol{F}_g$	Momentum equation	Eq. (2)
Governing equations of interface		
$\frac{\partial \phi}{\partial t}+\nabla\cdot(\phi \boldsymbol{u})=\nabla\cdot\left(M_\phi\nabla\mu_\phi\right)$	Cahn-Hilliard equation	Eq. (3)
Immersed Boundary Method		
$\boldsymbol{F}_b=2\rho\delta\boldsymbol{u}/\delta_t$	body force exerted by the solid wall	Eq. (4)
Wetting boundary conditions		
$\delta\phi=\sum_l\left[-2M_\phi\left(\left(\frac{\partial\mu_\phi}{\partial n}\right)_w-\frac{\partial\mu_\phi^*}{\partial n}\right)\right]D_{ij}\left(\boldsymbol{x}_{ij}-\boldsymbol{X}_B^l\right)\Delta s$	Correction term of ϕ	Eq. (5)
$\delta\mu_\phi=\sum_l\left[2\kappa\left(\left(\frac{\partial\phi}{\partial n}\right)_s-\frac{\partial\phi^*}{\partial n}\right)\right]D_{ij}\left(\boldsymbol{x}_{ij}-\boldsymbol{X}_B^l\right)\Delta s$	Correction term of μ_ϕ	Eq. (6)

3. Results and discussion

The conventional anode PTL design presents a challenge with the anode catalyst layer pressure exceeding that of the flow channel, necessitating liquid water to overcome backpressure for traversal. Even with baffles in the flow channel, this pressure distribution remains unchanged. We explored replacing the anode PTL with structures featuring straight and Tesla through-holes, but the backpressure persisted. Baffles were used to isolate the bottom of the anode PTL and redirect liquid into its interior, resulting in an S-shaped pressure distribution. This promotes liquid inflow and facilitates bubble detachment from the anode catalyst layer, significantly reducing gas content within the PTL. Quantitatively, the time for oxygen bubbles to traverse from the anode catalyst layer to the flow channel is 0.05 - 0.07 seconds for the straight and Tesla through-hole PTL with baffles, removing gas 9.9-14.2 times faster than traditional PTL.

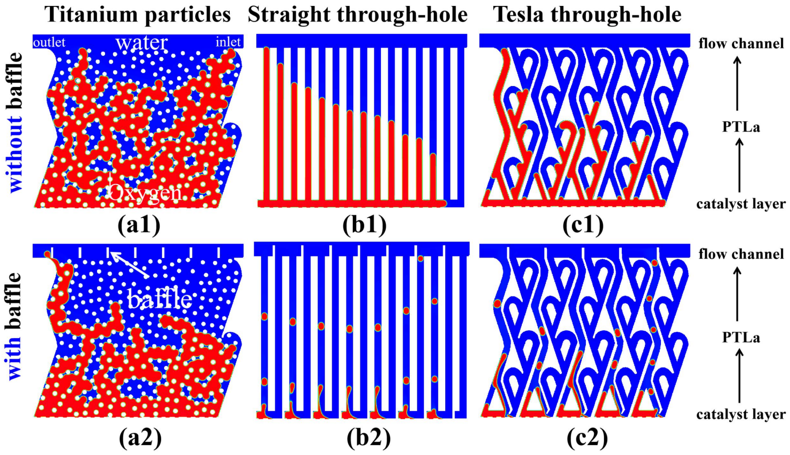

Figure 1. Gas distributions in different anode PTL .

4. Conclusions

In this study, we developed the Immersed Boundary Method - Phase Field Model - Lattice Boltzmann Method (IBM-PFM-LBM) to investigate oxygen blockage in the anode PTL at the titanium particle level. Our approach accurately replicates the variations in observed oxygen saturation in experimental settings. We found that the rheological behavior of the bubble is primarily influenced by the throat under high current density conditions. Optimizing the anode PTL has proven to be more effective in enhancing gas removal compared to optimizing operational conditions. Consequently, we proposed two new PTL designs: a straight through-hole PTL with baffles and a Tesla through-hole PTL with baffles. The bubble removal rate of these two PTL designs is 9.9 to 14.2 times faster than that of the PTL with titanium particles. Therefore, this study holds significant importance for further optimizing the design and improving the performance of anode PTL in PEM water electrolysis.

References

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Keywords

Porous transport layer; Structure optimization; Oxygen removal; Lattice Boltzmann Method.