

Supplementary Information

LBM Simulation of Water Removal and Heat Accumulation in PEMFCs: Influence of GDL Multilayering and Determinants of Dynamic Reaction Rates

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Model validation

Model Validation of diffusion and reactive transport

To verify the accuracy of the mass transfer in the LBM-based model, diffusion and reactive transport are simulated in a rectangular domain following Kang et al. ^[1,2], enabling direct comparison with analytical solutions. The simulation domain has dimensions $L \times W$. A reactive boundary is imposed at the top ($y = W$), while a constant concentration ($C_0 = 1.0$) is prescribed at the left boundary ($x = 0$). Both the bottom ($y = 0$) and right ($x = L$) boundaries are specified as no-flux and non-reactive. The governing equations and boundary conditions are given by:

$$\frac{\partial^2 C(x,y)}{\partial x^2} + \frac{\partial^2 C(x,y)}{\partial y^2} = 0 \quad (1)$$

$$C(0,y) = C_0 \quad (2)$$

$$\frac{\partial C}{\partial x} \Big|_{x=L} = 0 \quad (3)$$

$$\frac{\partial C}{\partial y} \Big|_{y=0} = 0 \quad (4)$$

$$-D \frac{\partial C}{\partial y} \Big|_{y=W} = k(C_W - C_{eq}) \quad (5)$$

$$Da = \frac{kl}{D} \quad (6)$$

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where $L = 1.0 \text{ cm}$, $W = 0.8 \text{ cm}$; the Damköhler number Da is set to 48, indicating the relative strength of reaction to diffusion; k is the reaction rate constant, set to $4.8 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$; l is the reaction boundary length, set to 1.0 cm ; and D is the diffusion coefficient, set to $1.0 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$. Fig. S1 compares the steady-state concentration profile from this study with the analytical solution and shows a discrepancy below 3%, confirming the accuracy of the diffusion and reactive transport simulation.

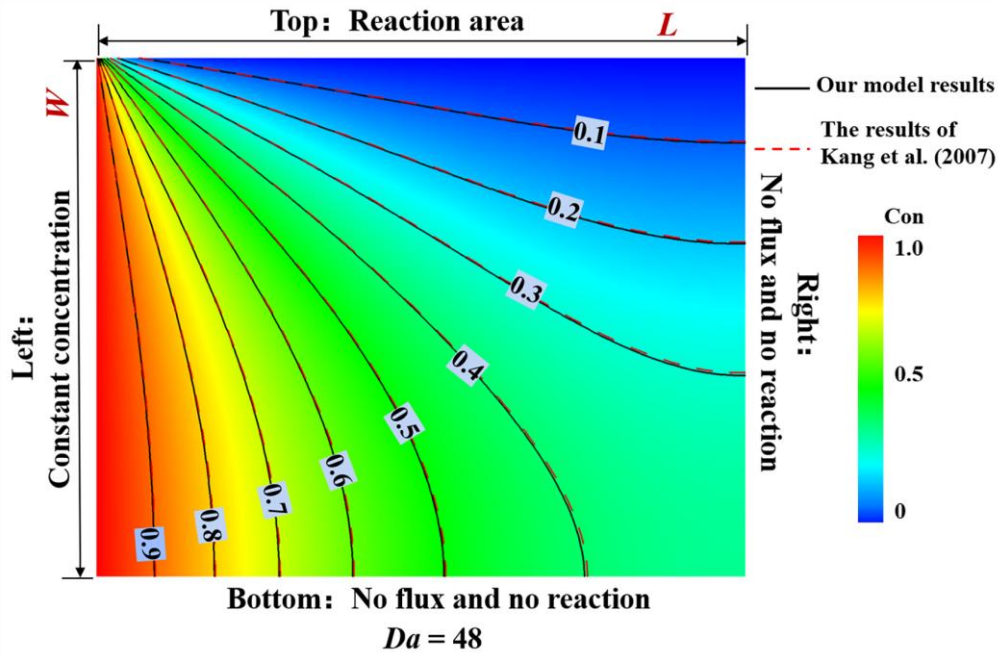


Fig. S1. Validation of the diffusion and reactive transport with $Da = 48$.

Validation of heat transport

To validate the accuracy of heat transport in the LBM-based model, a heat transport test was conducted in the channel and compared with the corresponding analytical solution^[3]. The simulation domain consisted of 200×120 lattice nodes. The top and bottom boundaries were maintained at constant temperatures of $T_H = 400 \text{ K}$ and $T_C = 380 \text{ K}$, while periodic boundary conditions were applied at the left and right boundaries. As shown in Fig. S2a, the LBM simulation yields the steady-state temperature distribution, while Fig. S2b further demonstrates that the temperature profile varies linearly along the vertical direction. The numerical results obtained from the LBM model agree well with the analytical solution.

Subsequently, heat transport in a non-uniform GDL structure was further simulated. A GDL

structure with geometric parameters similar to those reported by Jiao et al. ^[4] was generated using the GDL reconstruction algorithm adopted in this work, and the local temperature distribution was evaluated under the same initial and boundary conditions. Fig. S2c compares our model results with the local temperature distribution reported by Jiao et al. ^[4] in a non-uniform GDL. The results show that the overall temperature variation trend is consistent with the reported data, while local differences remain because the reconstructed GDL structure generated by our model has the same macroscopic parameters as those reported by Jiao et al. ^[4] but different local structural features. The overall average error remains below 5%, thereby confirming the reliability of the heat transport simulation.

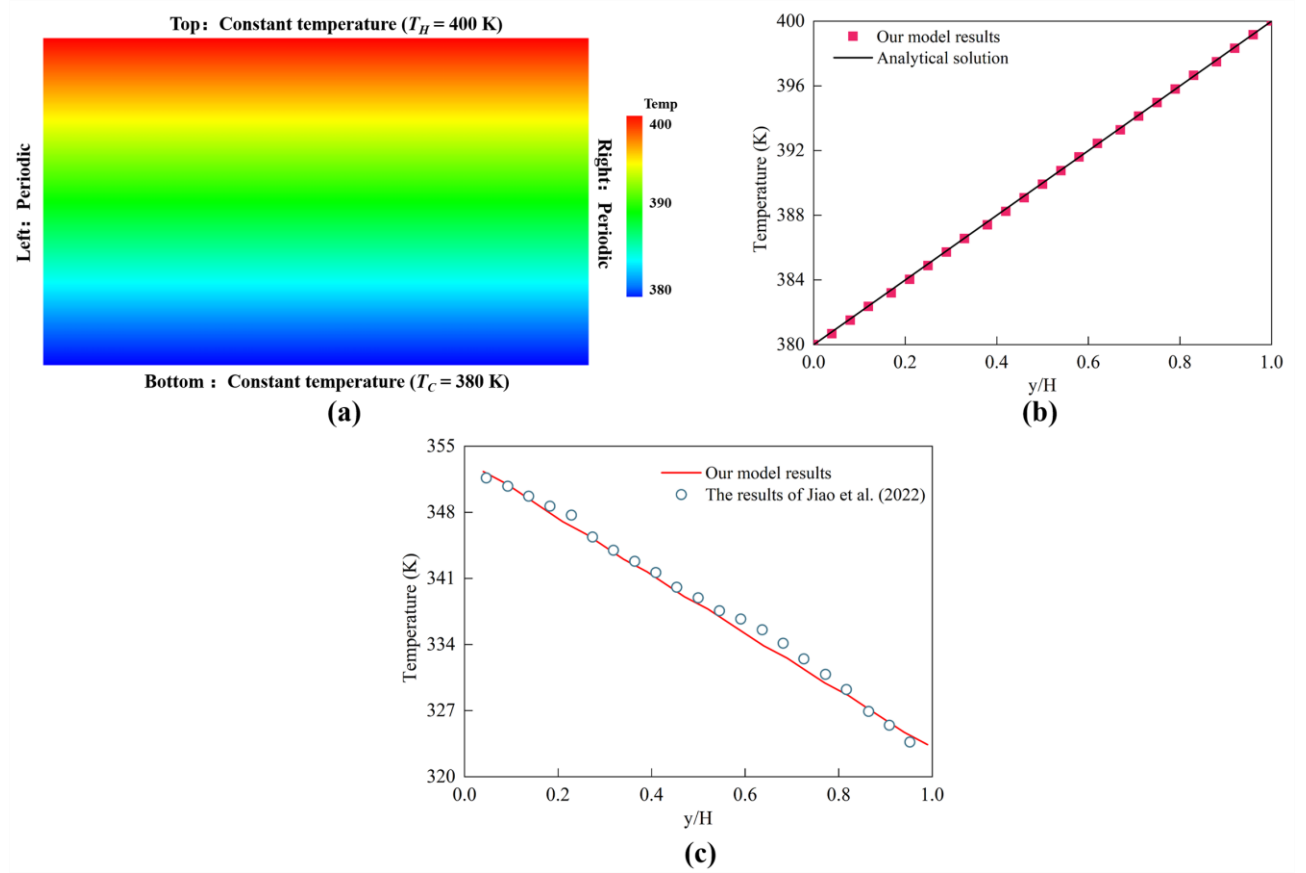


Fig. S2. Validation of heat transport. (a) Temperature distribution in the channel, (b) comparison of our model results with the analytical solution in the channel, and (c) comparison of our model results with the results reported by Jiao et al. ^[4] in a non-uniform GDL.

Validation of spurious velocity

To validate the accuracy of the two-phase flow simulation in the LBM model, the spurious velocity near the phase interface was evaluated. Numerous studies have demonstrated that the MRT

LBM model can effectively suppress spurious velocity near phase interfaces ^[5]. In this work, a two-dimensional simulation domain with 100×100 lattice nodes. As shown in Fig. S3a, the steady-state droplet configuration indicates that spurious velocity is primarily concentrated near the phase interface. Fig. S3b further quantifies the magnitude distribution of spurious velocity and shows a maximum value of approximately 0.00068, which is below the threshold of 0.0016 ^[5] for sufficiently small and stable spurious currents, thereby indicating a negligible impact on interface motion in the present simulations.

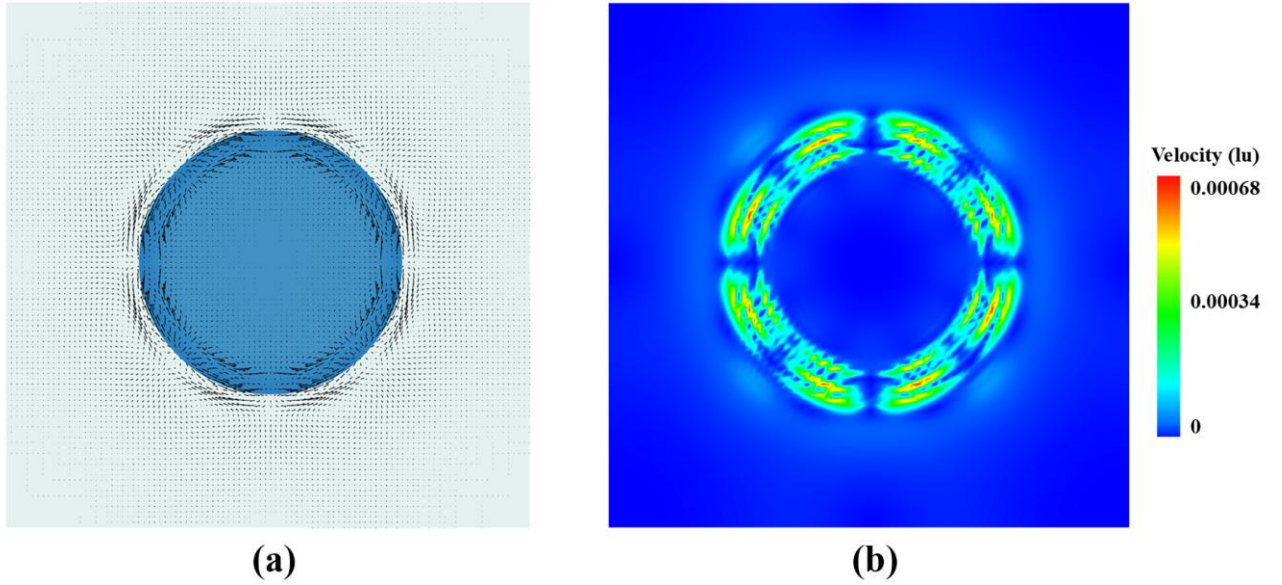


Fig. S3. Steady-state distributions of (a) droplets and (b) spurious velocity magnitude.

Young-Laplace law validation

Given the interactions within the multicomponent system, the Young-Laplace law is employed to simulate the static bubble test, which characterizes the proportional relationship between the pressure difference and the radius of curvature, thereby further validating the accuracy of the model ^[6]. It is expressed as follows:

$$p_i - p_0 = \frac{\sigma}{R} \quad (7)$$

where p_i and p_0 denote the steady-state pressures of the different phases; σ is the interfacial tension, and R is the curvature radius of the interface. The phase interface is defined as:

$$\phi = \frac{\rho_i - \rho_0}{\rho_i + \rho_0} \quad (8)$$

where ϕ denotes the order parameter associated with the phase interface, and $\phi = 0$ defines the interface location. Fig. S4 presents the droplet test results, showing a linear relationship between droplet radius and interfacial tension with a slope of 0.22. The discrepancy between the LBM results and the Young-Laplace prediction remains below 3%, confirming that the model reproduces an accurate capillary pressure response to interfacial curvature.

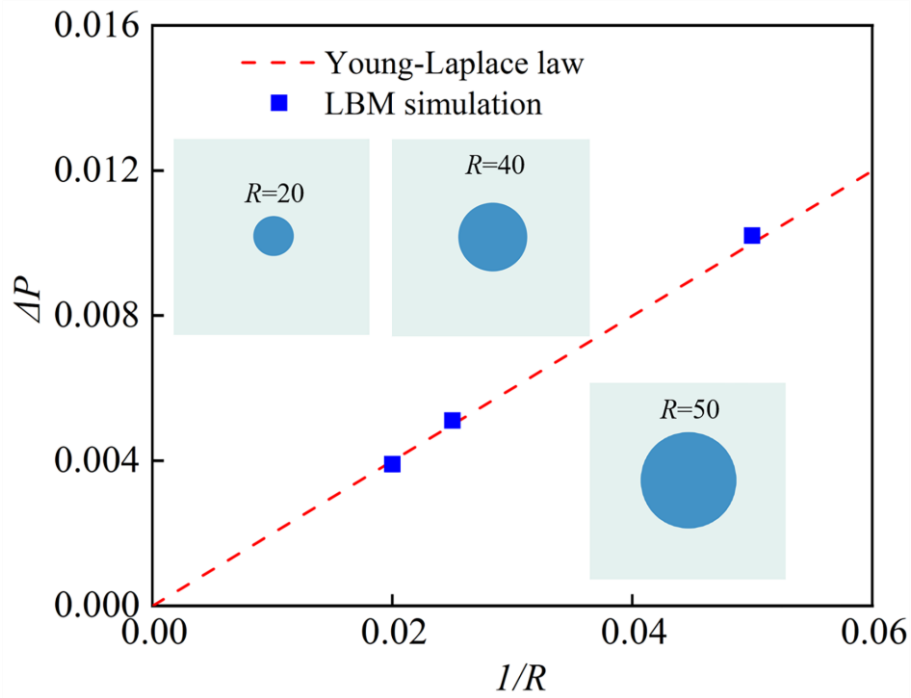


Fig. S4. Validation of the bubble test and the Young-Laplace law.

Validation of fluid-solid contact angle

The wettability of the multicomponent fluid on the electrode surface varies, leading to different contact angles. This behavior is governed by adjusting the parameter G_a^{as} . When $G_a^{as} > 0$, the contact angle exceeds 90° , indicating hydrophobicity. Conversely, when $G_a^{as} < 0$, it falls below 90° , indicating hydrophilicity [7]. Accordingly, the model establishes a direct relationship between G_a^{as} and the contact angle. As illustrated in Fig. S5, a semicircular droplet is initialized on the bottom wall. By varying G_a^{as} , the resulting indirect contact angle at the droplet wall interface is measured to quantify the relationship between G_a^{as} and the fluid-solid contact angle. This validation confirms that the model reproduces the prescribed wettability, which directly affects capillary entry and water distribution in a hydrophobic GDL.

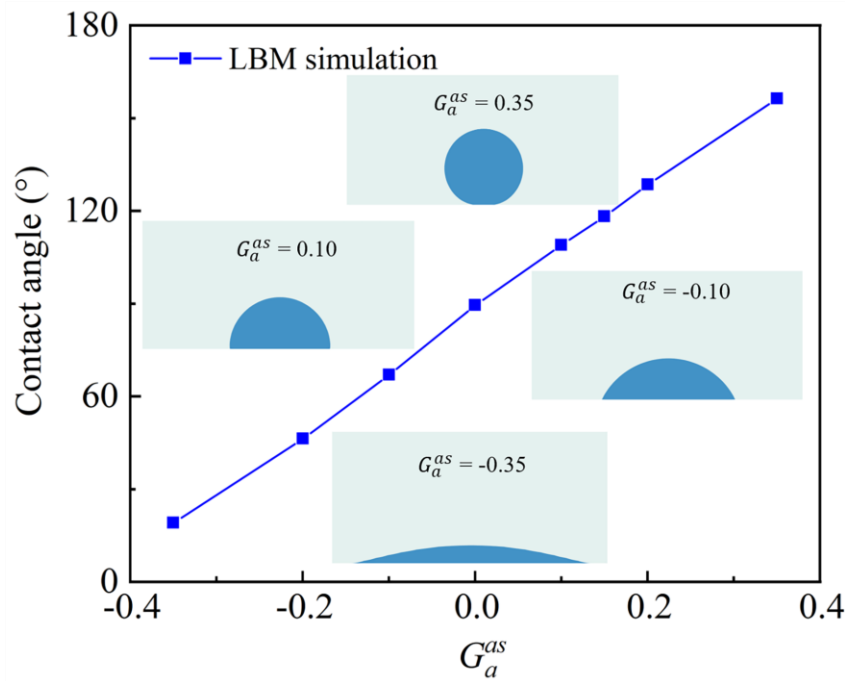


Figure S5. Validation of the different fluid-solid contact angle.

References

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