



1-1- Two Phase Simulation of Droplets Motion in Cathode Channels and Manifolds of Polymer Electrolyte Membrane Fuel Cell

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ABSTRACT: Polymer electrolyte membrane fuel cell with a combination of oxygen and hydrogen and production of water converts the chemical energy of the fuel directly and through an electrochemical reaction to electrical energy. One of the most crucial issues for commercializing this technology is water management. In the present study, the motion of liquid droplets that emerged in the gas flow channels with inlet and outlet manifolds is investigated. Due to the small dimensions of these channels, the balance of surface adhesion and other dynamic forces influence the flow of fluid, therefore, the semi-empirical Hoffman model with a two-phase flow method for simulating physics in an applied geometry including gas flow manifolds are used. The effect of tapering the manifold cross-section on the liquid water droplets is also investigated. The physical model used for the dynamic contact angle is validated with data from an experimental study. Simulation results show that by changing the geometry of the input and output manifolds, the problem created in conventional geometry, which causes the obstruction of the last channel due to the accumulation of liquid water, will be resolved, thereby improving the geometry will improve the water management in the channels.

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1- Introduction

Fuel cell technology in which hydrogen and oxygen during a chemical reaction convert into electricity and heat is one of the best options for generating electrical energy in the future. But similar to all growing technologies, there are some challenges toward development of its social penetration. One of the most important issues that many researchers are engaged with is the management of liquid water in the fuel cell [1]. Some researchers [2] have proposed efficient techniques for preventing liquid water to be emerged in the fuel cell entrance manifold and consequently to fuel cell gas channels. However, since the appearance of liquid water in the gas flow field is unavoidable, it is necessary to examine the dynamics and behavior of water and the effects of this movement in the fuel cell [3]. Therefore, in the present work, after validating the applied model with related experimental data, the dynamic behavior of liquid droplets in a common gas flow field is investigated. The dynamic contact angle of droplets is considered using the Huffman function model, which considers physical and fluid flow characteristics and was neglected in previous studies. Also, the motion of the droplet dynamics in applied geometry, which includes manifolds of gas flow field in Polymer Electrolyte Membrane (PEM) fuel cell, has been studied. Finally, a novel design for improving liquid water management in the manifolds of gas flow field is introduced.

2- Numerical Methodology

Because of the nature of the two-phase flow that concerned

with this problem, the volume of fluid method has been used to solve the governing equations [3]. This method is used to simulate the flow regime with unmixable fluids in an unsteady state flow. The key feature of this technique is its ability to take into account the effects of surface tension. Huffman function [5] is used as the model of the contact angle or the hysteresis of the contact angle. First, the value of capillary number is calculated using the liquid phase properties and the contact line speed of this phase from Eq. (1).

$$Ca = \frac{\mu V}{\sigma} \quad (1)$$

Then the dynamic contact angle is obtained as an indicator of the dynamic effects of flow based on the capillary number and static contact angle as an index of surface adhesion effects as follows:

$$\theta_D = f_{Hoff} [Ca + f_{Hoff}^{-1}(\theta_e)] \quad (2)$$

where Hoffman function is defined as Eq. (2):

$$f_{Hoff}(x) = \arccos \left\{ 1 - 2 \tanh \left[5.16 \left(\frac{x}{1 + 1.31x^{0.99}} \right)^{0.706} \right] \right\} \quad (3)$$

The written code estimates the numerical value of the inverse Huffman function by using the value of the static contact

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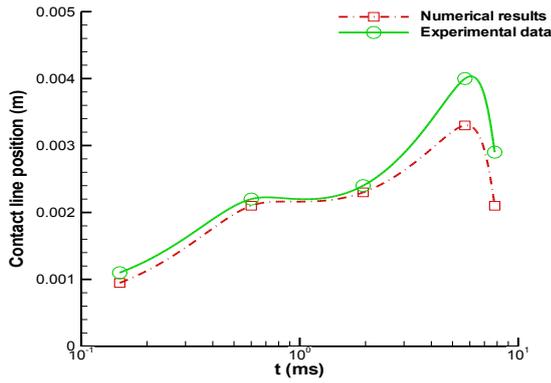


Fig. 1. Validation with experimental data

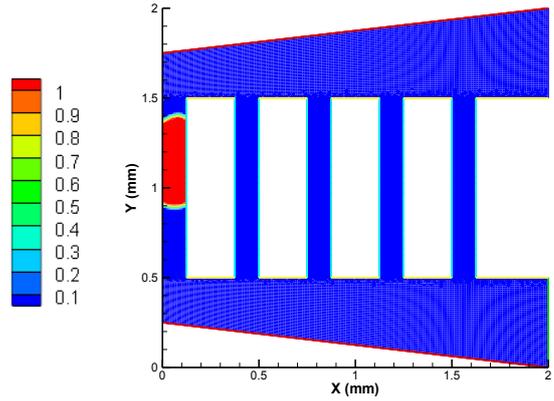


Fig. 3. Moving of droplets in the corrected flow field

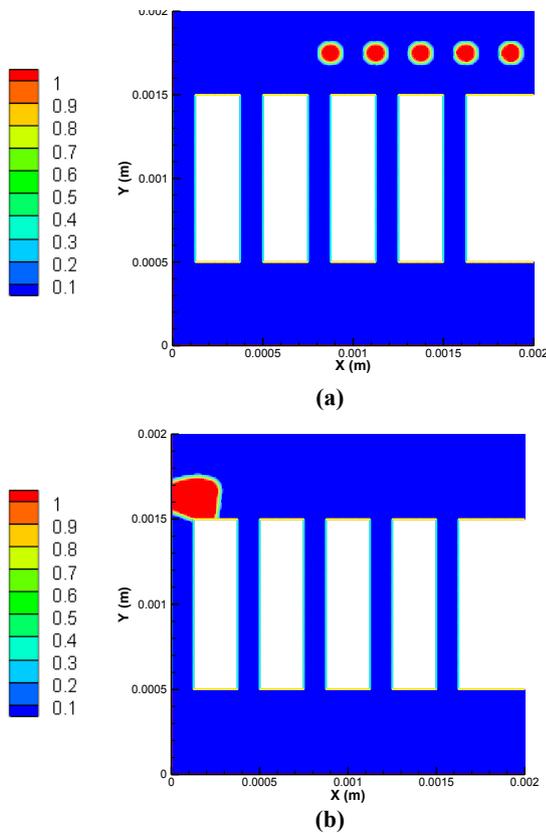


Fig. 2. Moving of five droplets in the initial flow field

angle, then it sums obtained amount with the value of capillary number so the dynamic contact angle is estimated and the boundary condition of the wall in the code will be applied. Of course, regarding the transient nature of the problem, the above-mentioned process must be iterated at each step to update the new value of dynamic contact angle.

3- Results and Discussion

First, according to the work carried out in reference [4] and the preliminary speculation of the limits of suitable grid density, the dependency of the numerical grid was

investigated. Then, in order to ensure the correctness of the simulation and the applied model, the results were validated with the results presented in Ref. [5]. In Fig. 1, the result of this process is presented in the form of a comparison of the position of the contact line position for the experimental data and simulation performed by implementing the Hoffman function for the effect of the contact angle hysteresis as the boundary condition of walls and the volume of fluid method for the two-phase model. As can be seen, the results initially are in good agreement with experimental data, but in continue a limited difference emerges. The most important factor makes this difference caused is the difference between the two-dimensional simulation and the actual three-dimensional conditions in the experiment.

Figures 2 and 3 show the initial and modified geometries of the problem, respectively. Figure 2a shows the initial arrangement and Fig. 2b shows the final state of droplets. After moving a little towards the end of entrance manifold, single droplets stick to each other and form a larger one. This larger droplet moves toward the last channel by encountering the wall opposite the manifold. As a result, this large droplet does not have the ability to pass through the channels. That is, the last channel is blocked. Naturally, this problem will exacerbate flooding if water continues to flow into the structure. This led to the idea of a new design of the flow field.

The flow of five drops in the modified geometry is shown in Fig. 3. The expansion and contraction ratio is considered 0.5 in both input and output manifolds. It can be seen that the geometric modification changes the behavior of the formed droplet. It should be noted that the modification of geometry in both the inlet and outlet manifolds causes this function, and if the geometry of each of them is changed lonely, the problem of channel obstruction will remain. On the other hand, the slope created in the manifold should be in the direction of the movement of the fluid.

4- Conclusions

The gas-liquid two-phase flow of five pre-embedded droplets in parallel straight channels with the inlet and outlet manifolds is simulated. For this purpose, the mass and momentum conservation equations are solved using the volume of fluid method and considering the Hoffman function

for modeling the dynamic contact angle. The results show that in the moving of five drops in the flow field of parallel channels and common geometry of manifolds, with merging of droplets and increasing the diameter of them, the dynamic of their motion in the flow field is changed and due to the effects of surface tension, the last channel gets blocked. But by changing the geometry of the input and output manifolds, the problem will resolve. As a result, improving geometry improves water management in the flow field.

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