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Short Communication

Direct numerical simulation of two-phase turbulent flow in fuel cell flow channel

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ABSTRACT

For high-performance low-temperature fuel cells (e.g. hydrogen proton exchange membrane fuel cell for powering vehicles), significant amount of reactant needs to be supplied, leading to turbulent two-phase flow, which is largely ignored in previous studies. In this study, a direct numerical simulation (DNS) model of the two-phase turbulent flow in fuel cell flow channel is developed with a modified volume-of-fluid (VOF) approach for tracking the air/water interface. The turbulent flow inlet of the two-phase DNS model is obtained from a validated single-phase DNS model. By resolving the whole range of spatial and temporal scales of turbulence, the results of the two-phase DNS model show that the deformation of water droplet is asymmetric and broken into small pieces/films, and is significantly different from the laminar and the corresponding $k - \epsilon$ models. It is suggested that the turbulence effect on the two-phase transport in fuel cell flow channel is significant and needs to be considered for water management by using the DNS model.

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Introduction

Low temperature fuel cells (operating temperature $< 100^\circ \text{C}$), such as the well-known proton exchange membrane fuel cell (PEMFC) and the fast-growing alkaline anion exchange membrane fuel cell (AEMFC), possess many outstanding features such as high power density, rapid load response and efficient energy conversion, and have attracted considerable attentions in a wide range of applications. However, for such low temperature fuel cells, the product water may exist in liquid state and block the flow channel and electrode, causing serve mass transport loss.

Significant efforts have been made by researchers to investigate the two-phase transport characteristics in fuel cell flow channel. Experimental observation techniques such as the direct visualization [1–4], 3D neutron tomography [5,6] and X-ray imaging [7,8] have been conducted to visualize the two-phase transport behaviors in flow channel and gas diffusion layer (GDL). However, such experiments often have high requirements on the facilities.

Alternatively, two-phase numerical models can also be used cost-effectively to investigate the water transport characteristics in fuel cell. Among the different two-phase models, the volume-of-fluid (VOF) method has been used by many researchers mainly because of its ability for interface tracking

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between liquid water and air [9]. By using the VOF method, Jiao et al. [10,11] investigated the air–water flow in parallel and serpentine flow channels; Zhu et al. [12] considered a 2D flow channel to explore the water emerging process from GDL pore to flow channel; Qin et al. [13,14] placed a hydrophilic plate and a needle in a flow channel and analyzed its effect on water removal; and Park et al. [15] and Wu et al. [16] reconstructed the 3D fibrous porous structures of GDL, and studied the effect of GDL microstructure on liquid water transport behavior.

Generally, most of the previous models only considered the channel flow to be laminar, by claiming that the inlet flow velocity is low [9,17]. However, with the significant performance improvement of fuel cell in recent years, especially for PEMFC (e.g. current density even higher than 3 A cm^{-2}) [17,18], and considering the large reaction area for high-power fuel cell stacks (e.g. hydrogen PEMFC stacks for powering vehicles), significant amount of gas reactant, especially for air, is needed for each single cell in a stack, which may lead to very high flow velocity and turbulent flow characteristics.

Taking a PEMFC cathode as an example, by considering the following parameters: reaction area 300 cm^2 , current density 3 A cm^{-2} (high load operation), stoichiometry ratio 2, temperature 80° C , and flow channel cross-section $1 \text{ mm} \times 1 \text{ mm}$ (the channel height is generally in the range of $0.4 \text{ mm}–1 \text{ mm}$ [19–21]), the inlet velocity of air is nearly 500 m s^{-1} for each single cell, and the corresponding Reynolds number is about 23,300, which is apparently turbulent flow. For three-serpentine or five-serpentine parallel design, it is turbulent flow in each parallel channel. For straight-parallel design with more parallel channels, it is turbulent flow in the manifolds; and if the non-uniform flow among the different single cells in a stack (or among the different parallel channels in a single cell) together with air humidification are considered, the Reynolds number is expected to be higher in some of the parallel channels, in which the flow might be turbulent as well. Therefore, it is necessary to investigate the two-phase turbulent flow characteristics in fuel cell flow channel.

To the best of the authors' knowledge, there have been little studies investigating the turbulent two-phase (air/water) transport in fuel cell flow channel [9,17]. Since the turbulent flow is highly random and has significant spatial and temporal variations, which may have significant effects on the structure of air/water interface, the traditional turbulent models that cannot resolve all the turbulent effects, such as the $k-\epsilon$ and large eddy simulation (LES) models, may be improper to be used with the interface tracking methods (e.g. VOF model). On the other hand, the direct numerical simulation (DNS) model resolving the whole range of spatial and temporal scales of turbulence is probably the most suitable method. So far, for turbulent channel flows (including the fuel cell and all the other flow channels), the DNS method was mainly used for

bubbly flow simulations [22–26], and the water droplet transport in air was largely ignored.

Therefore, in this study, a two-phase DNS model is developed and used to investigate the effect of all the turbulent fluctuations on the liquid water droplet transport process in a fuel cell flow channel. A modified VOF approach [27] is used to capture the interface of the two phases. A laminar and the corresponding $k-\epsilon$ simulations [27] are also conducted to compare with the DNS results.

Numerical model

Governing equations

Single-phase turbulence flow

The single-phase turbulent flow is considered to be fully developed and incompressible in a square duct of $6.2 \text{ mm} \times 1 \text{ mm} \times 1 \text{ mm}$, as described in Table 1. The governing equations are the continuity and Navier–Stokes equations:

$$\nabla \cdot \vec{U} = 0 \quad (1)$$

$$\frac{\partial \vec{U}}{\partial t} + \nabla \cdot (\vec{U}\vec{U}) = -\nabla p + \nu \nabla^2 \vec{U} + F_i \quad (2)$$

The Cartesian coordinates are x , y and z with x being the flow direction and y – z the cross-section plane. p is the fluctuating pressure, and ν the kinematic viscosity. F_i is the mean part of the pressure gradient field, which is used to drive the flow by setting its streamwise component to a non-zero constant value. For convenience, the friction Reynolds number is defined as $Re_\tau = u_\tau H / \nu$ with $u_\tau = \sqrt{\tau_w / \rho}$ being the friction velocity, where τ_w is the wall shear stress averaged in time for the four side walls, ρ the density and H the width of flow channel. In this study, the friction Reynolds number $Re_\tau = 300$, and the average inlet velocity is about 60 m s^{-1} . Because the flow is driven by a constant pressure gradient along the flow direction, dP/dx , the average value of the friction velocity on the four side walls of flow channel is given as

$$u_\tau^2 = -\frac{1}{4} H \frac{dP}{dx} \quad (3)$$

Two-phase turbulent flow

A modified VOF approach with a combination of two-fluid formulation and the conventional VOF method [27] is adopted to improve interface resolution and has been validated in Ref. [28]. The governing equation for a phase fraction γ can be written as

$$\frac{\partial \gamma}{\partial t} + \nabla \cdot (\vec{U}\gamma) + \nabla \cdot [\vec{U}_r \gamma (1 - \gamma)] = 0 \quad (4)$$

Table 1 – Geometrical and computational parameters.

Quantity	Mesh number (x, y, z)	Time step	Channel dimension
Single-phase DNS	$120 \times 140 \times 140$	$1 \times 10^{-8} \text{ s}$	$6.2 \text{ mm} \times 1 \text{ mm} \times 1 \text{ mm}$ (x, y, z, respectively)
Two-phase DNS	$380 \times 140 \times 140$	$1 \times 10^{-8} \text{ s}$	
Two-phase $k-\epsilon$	$360 \times 60 \times 60$	$2 \times 10^{-8} \text{ s}$	
Two-phase laminar	$200 \times 40 \times 40$	$5 \times 10^{-8} \text{ s}$	

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