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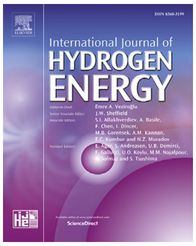
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Interface resolving two-phase flow simulations in gas channels relevant for polymer electrolyte fuel cells using the volume of fluid approach

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ABSTRACT

With the increased concern about energy security, air pollution and global warming, the possibility of using polymer electrolyte fuel cells (PEFCs) in future sustainable and renewable energy systems has achieved considerable momentum. A computational fluid dynamic model describing a straight channel, relevant for water removal inside a PEFC, is devised. A volume of fluid (VOF) approach is employed to investigate the interface resolved two-phase flow behavior inside the gas channel including the gas diffusion layer (GDL) surface. From this study, it is clear that the impact on the two-phase flow pattern for different hydrophobic/hydrophilic characteristics, i.e., contact angles, at the walls and at the GDL surface is significant, compared to a situation where the walls and the interface are neither hydrophobic nor hydrophilic (i.e., 90° contact angle at the walls and also at the GDL surface). A location of the GDL surface liquid inlet in the middle of the gas channel gives droplet formation, while a location at the side of the channel gives corner flow with a convex surface shape (having hydrophilic walls and a hydrophobic GDL interface). Droplet formation only observed when the GDL surface liquid inlet is located in the middle of the channel. The droplet detachment location (along the main flow direction) and the shape of the droplet until detachment are strongly dependent on the size of the liquid inlet at the GDL surface. A smaller liquid inlet at the GDL surface (keeping the mass flow rates constant) gives smaller droplets.

Introduction

With the increased concern about energy security, air pollution and global warming, the possibility of using polymer electrolyte fuel cells (PEFCs) in future sustainable and renewable energy systems has achieved considerable momentum [1–3]. The principle on which the fuel cell (FC) technology is based dates back to 1838 [4–6]. The PEFC has emerged as the most viable fuel cell type for automotive and

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Nomenclature

a	VOF function (fraction of liquid)
$\mathbf{F}$	source term, N/(m^{3}s)
$\mathbf{g}$	gravitational acceleration, m/s^2
m	mass transfer source term, mol/s or kg/s
$\mathbf{n}$	normal vector
p	pressure, Pa
R	local curvature of the gas-liquid interface
S	source term, mol/s or kg/s
t	time, s
$\mathbf{t}$	unit vector
u	velocity in x direction, m/s
$\mathbf{v}$	velocity vector
v	velocity in y direction, m/s
V	volume, m^3
w	velocity in z direction, m/s
θ	contact angle, ° or rad
γ	surface tension, N/m
ρ	density, kg/m^3
μ	dynamic viscosity, Pa s
κ	surface curvature

Subscripts and Superscripts

CV	computational volume
g	gas phase
k	phase k
l	liquid phase
q	phase q
w	wall
x,y,z	coordinate system

Abbreviations

CFD	computational fluid dynamics
CSF	continuum surface force
FC	fuel cell
GC	gas channel
GDL	gas diffusion layer
MPL	microporous layer
PEFC	polymer electrolyte fuel cell
VOF	volume of fluid

some portable applications, and also has potential back-up power unit applications due to its high power density, low operating temperature and comparative simplicity of construction [7–9]. In spite of engineering progress and scientific advances, over the last few decades, the commercialization of PEFCs remains unrealized, owing primarily to: (1) technical problems relating mainly to water management (2); high prices of materials and components and (3) the fragility of membranes [2,7,10–12] issues. The challenge in understanding water management lies mostly in coupled heat and mass transfer, the two-phase multi-component flow involving phase-change in porous media, the complex relationship between water content and cell performance as well as interactions between the gas channel (GC) and the gas diffusion layer (GDL). Water generated by the electrochemical reactions often condenses into liquid form, potentially flooding the GC, the GDL, the micro porous layer (MPL) and the catalyst layer. Insight into the fundamental processes of liquid water transport and evolution is still not complete, preventing further FC development [1,9,10,13,14].

Computational fluid dynamics (CFD) models make it possible to reduce the number of experiments needed for cell design and development, and only a limited amount of tests are then required to validate the accuracy of the models. Modeling can also be used to confirm experimental results and conclusions [9,15,16]. Various assumptions have to be made while developing CFD models [10,17,18].

A typical PEFC flow field consists of a series of mini/microchannels. The endless removal of liquid water from the cathode channels is a critical issue, as relatively large water droplets forming in the channels can cause flooding, thereby blocking the transport of gaseous oxygen to the active sites. This phenomenon results not only in an uneven current distribution, substantial loss of performance, but also, unstable operation and enhanced degradation rates [7,14,19]. Liquid water may break through at various locations to form droplets, for example, at the GDL surface. Proper GC geometry and wettability modification of the channel walls can enable water removal with a moderate pressure drop [20]. When the momentum of the gas in the GC overcomes the surface tension, the droplets detach via one or more of the following three flow patterns: (1) slug flow, (2) mist flow or (3) film/corner flow along the channel wall [21].

The aim of this work is to obtain an increased understanding of the impact of the size and location of the liquid inlet at the GDL surface, the wall and GDL surface contact angles as well as the gas velocity, for gas channels relevant for PEFCs. CFD calculations, in OpenFOAM [22,23], with the volume of fluid (VOF) approach [24–27] are used to be able to resolve the liquid/gas interface. A model describing one straight channel with one gas inlet, one liquid inlet (at the GDL surface) and one two-phase outlet is developed. The uniqueness of this work includes the systematic investigation of the importance of the size and location of the GDL surface liquid inlet. Additionally, a study is performed focusing on the contact angle of the GC wall as well as the GDL surface. VOF simulations of PEFC channels and/or GDLs require high performance computing, i.e., it is a relatively new research field and with significant potential, as the supercomputers continues to improve in performance. Existing flow pressure drop correlations and pattern maps for two phase flow in mini/microchannels [28,29] may or may not be applicable to GCs, due to one side wall being porous, with the resulting interaction between the GC and GDL.

Mathematical model

The VOF model [30] is an interface-resolving method and has become a popular methodology for solving two-phase flow phenomena within PEFCs [3,25,26,30–40]. With the VOF approach, the interface between the phases is tracked by the volume fraction of liquid water at the computational cell volume schemes [25,30–33]. According to the VOF approach, in each cell of a mesh, only one value for each dependent variable defines the state. A function a is introduced whose value is unity at any location occupied by liquid phase, and otherwise zero [26]:

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