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Comparisons and validations of contact angle models

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ABSTRACT

In the numerical simulation of water management for proton exchange membrane fuel cells (PEMFCs), the static contact angle (SCA) model is generally used. However, an empirical correlation for dynamic contact angle (DCA), known as Hoffman function or Kistler's law, was recently employed to numerically simulate the droplet behaviors either in a microchannel or on a surface. In this paper, for the first time, a DCA evolution map is created based on Hoffman function and related experiments to better understand the DCA evolving mechanism; based on this evolution map, the Advancing-Receding DCA (AR-DCA) model is proposed and explained, in addition to the Advancing DCA (A-DCA) model that is based on the original Hoffman's experiments; using user defined function (UDF), the A-DCA and AR-DCA models are implemented with Volume of Fluid (VOF) method in ANSYS Fluent; a series of numerical simulations are conducted with the SCA, A-DCA and AR-DCA models for droplet impact on horizontal and inclined surfaces; the validations of these contact angle models are performed, qualitatively and quantitatively, by comparing the numerical simulation results with the corresponding experimental results from the literature. It is indicated that the AR-DCA model can better simulate the droplet deformation and evolvement, showing its potential for the DCA simulations in a more complex gas-liquid flow domain such as the cathode of PEMFCs.

Introduction

Liquid water management is still one of the most challenging issues for the commercialization of proton exchange membrane fuel cells (PEMFCs). Numerical modeling and simulation can effectively predict liquid water behaviors in gas channels, which provide viable approaches to the investigation of two-phase flow in PEMFCs. Contact angle, as a crucial parameter in the boundary conditions for numerical simulation, has significant effects on droplet deformation and evolvement. However, from available literature, it is known that the static contact angle (SCA) is usually considered in PEMFC modeling (e.g., the previous works conducted by Zhou et al. [1–6], Zhu et al. [7,8], Qin et al. [9,10], Ding et al. [11–13], etc.), and the dynamic contact angle (DCA) model has not been reported for PEMFC simulations mainly because of the complex flow field design.

In order to apply DCA in PEMFC simulations, first, it is very important to thoroughly understand the fundamentals of DCA and its correlations.

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Nomenclature

Ca	capillary number
D	initial droplet diameter (mm)
d_0	droplet falling distance (mm)
F	shift factor
l	droplet spreading length (mm)
V	interface velocity (m s^{-1})
V_0	droplet initial velocity (m s^{-1})
V_i	droplet impact velocity (m s^{-1})
V_{cl}	contact line velocity (m s^{-1})
We	weber number
S	source term
f_{Hoff}	Hoffman function
f_{Hoff}^{-1}	inverse of Hoffman function
$\hat{n}$	surface normal
$\hat{n}_w$	unit vectors normal to the wall
$\hat{t}_w$	unit vectors tangential to the wall
s	phase volume fraction
$\vec{u}$	velocity vector (m s^{-1})

Greek symbols

α	inclined angle of surface (°)
γ	surface tension (N m^{-1})
θ	contact angle (°)
κ	surface curvature (m^{-1})
μ	dynamic viscosity (mPa s)
ρ	density (kg m^{-3})

Subscripts

LG	liquid/gas interface
SG	solid/gas interface
SL	solid/liquid interface
a	advancing
c	continuity
cl	contact line
d	dynamic
e	equilibrium
g	gas phase
l	liquid phase
m	momentum
r	receding
s	static

Abbreviations

A-DCA	advancing dynamic contact angle
AR-DCA	advancing-receding dynamic contact angle
DCA	dynamic contact angle
SCA	static contact angle
VOF	volume of fluid

Contact angle – definition

The contact angle, i.e., the angle between the liquid/gas interface and the solid surface (Fig. 1), plays an important role in gas-liquid dynamics. The value of the contact angle is determined by the relationship of interfacial energy among the three phases (gas, liquid, and solid) at the equilibrium state [14]. The state of equilibrium has the property of not varying so long as the external conditions remain unchanged [15]. Therefore, Young's equation [14] can be used to describe the contact angle:

$$\gamma_{LG}\cos\theta_e = \gamma_{SG} - \gamma_{SL} \quad (1)$$

where θ_e is the contact angle at equilibrium, and γ_{LG}, γ_{SG}, and γ_{SL} are the surface tension of the liquid/gas interface, the solid/gas interface, and the solid/liquid interface, respectively. In the case of a droplet resting on a flat surface, the contact angle is referred to as the static contact angle (SCA), θ_s. If a small enough amount of liquid is added to/removed from a drop, while the contact line does not move, the contact angle will increase/decrease. Before the contact line starts to move, the maximum contact angle is the advancing contact angle θ_a, whereas the minimum is the receding contact angle, θ_r. The contact angle θ_e is somewhere between θ_a and θ_r, and the difference between θ_a and θ_r, i.e., $(\theta_a - \theta_r)$, is usually defined as the contact angle hysteresis.

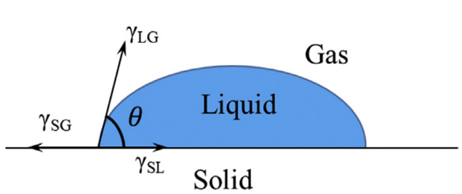

Fig. 1 – Definition of contact angle.

However, in many practical applications involving droplets, the surrounding gas will flow around and interact with the droplets, thus the contact angle is unlikely to stay at static equilibrium and will become DCA. In general, SCA is a property of the gas-liquid and surfaces. However, DCA is influenced by both gas-liquid and surface properties and the gas-liquid interactions. In gas-liquid two-phase flow modeling, as a critical parameter at the surface boundaries, DCA rather than SCA should be used.

Dynamic contact angle formulation – Hoffman function

Richard L. Hoffman is one of the pioneers in the experimental investigation of the advancing dynamic contact angle (A-DCA) [16]. Hoffman conducted a systematic study in flow regime where the viscous and interfacial forces play a dominant role on the interface shape. He built up a meniscus type of apparatus to obtain the advancing liquid-air interface with varying interface velocity through a glass capillary tube, and the liquid moved over a solid surface and displaced the gas. A microscope was utilized to view the interface and capture the images. The interface velocity was evaluated from the plunger velocity with a correction factor which is required due to the backflow of the liquid into the space between the plunger and the glass tube. The experimental data was obtained from five different liquid systems and the capillary number was ranged from approximately 4×10^{-5} to 35.4. By plotting the data from