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Numerical study of droplet dynamics in a polymer electrolyte fuel cell gas channel using an embedded Eulerian-Lagrangian approach

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HIGHLIGHTS

- We model the droplet dynamics on a PEFC cathode gas channel with a novel technique.
- A simple method to obtain interface curvature in two dimensions is given.
- Dynamic contact angle condition for droplets on rough surfaces is presented.
- Results can predict several variables of interest and agree with experimental data.

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ABSTRACT

An embedded Eulerian-Lagrangian formulation for the simulation of droplet dynamics within a polymer electrolyte fuel cell (PEFC) channel is presented. Air is modeled using an Eulerian formulation, whereas water is described with a Lagrangian framework. Using this framework, the gas-liquid interface can be accurately identified. The surface tension force is computed using the curvature defined by the boundary of the Lagrangian mesh. The method naturally accounts for material property changes across the interface and accurately represents the pressure discontinuity. A sessile drop in a horizontal surface, a sessile drop in an inclined plane and droplets in a PEFC channel are solved for as numerical examples and compared to experimental data. Numerical results are in excellent agreement with experimental data. Numerical results are also compared to results obtained with the semi-analytical model previously developed by the authors in order to discuss the limitations of the semi-analytical approach.

1. Introduction

Water management is a key limiting factor of PEFCs performance [1]. Water is produced by the oxygen reduction reaction (ORR) in the cathode catalyst layer (CL) of the fuel cell. At high current densities excess liquid water is evacuated through the pores of the gas diffusion layer (GDL). When it emerges from the pores into the gas channels it may form droplets, films or slug flows depending on the working conditions [2]. Interface conditions between the channel and the GDL remain largely unknown and continue to be a very active area of research [3]. The present study proposes a novel technique to improve the numerical analysis of droplet dynamics on the GDL surface.

There are several studies in the literature that investigate droplet dynamics using an analytical approach [4–6]. The authors recently proposed a semi-analytical model that improved previous treatments of drag and adhesion forces [7]. Although these models provide solutions with low computational cost, they oversimplify the phenomena by either using predefined droplet geometries or neglecting water-air interactions. For gravity-dominated flows, such as film or slug flows, analytical models cannot describe the geometry and therefore they cannot be used [7]. Surface tension and adhesion forces strongly depend on geometry. Contact angle hysteresis, i.e, the difference between advancing and receding angles, is used to predict droplet detachment [1,8]. An accurate description of the geometry is key to model droplet dynamics.

Numerical methods can be used to provide more accurate

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droplet dynamics predictions. Several studies in the literature study the phenomena using an Eulerian formulation together with the Volume of Fluid (VOF) method [9]. A review of two and three-dimensional droplet dynamics models based on the VOF method can be found in Ref. [10].

Previous numerical simulations based on the Volume of Fluid method implement the surface tension force using the Continuum Surface Force (CSF) as a volumetric force in the momentum equation [10–11]. The formulations rely upon an explicit treatment of the surface tension. This restricts the model to using extremely small time steps (governed by the time scale associated with the propagation of capillary waves) in order to achieve convergence [12]. This restriction is an important drawback for practical PEFC simulations. Additionally, VOF studies need very fine meshes to have an accurate description of the interface. This further increases the computational cost of the corresponding simulations.

An alternative to Eulerian models are the Lagrangian models, such as the one proposed by Saksono and Perić [13]. Saksono and Perić [13] proposed a variational formulation for the surface tension term. One of the advantages of Lagrangian models is that they can track exactly the water domain and its boundary. This formulation could be used to describe quasistatic and dynamic problems [14]. The application of the model presented in Ref. [13] is however restricted to the water domain. Air-water interactions were not studied. A multi-fluid model using a pure Lagrangian formulation was presented in Ref. [15]. Results showed that steady-state solution presented spurious velocities at the interface. Lagrangian models have the additional disadvantage that the domain has to be remeshed after each time step in order to avoid mesh degradation. In the context of PEFC gas channels, a model treating both the gas and the liquid droplets in a Lagrangian framework would have a large computational cost due to remeshing.

Recently, embedded Eulerian-Lagrangian formulations have been proposed [16–17]. This approach has been shown to be advantageous for fluid-fluid problems as it restricts the mesh moving and remeshing to the liquid domain, while maintaining a fixed mesh for the gas. This approach is very well suited to study liquid drops in fuel cell channels since it allows for:

a) natural tracking of the liquid-gas interface
b) efficient partitioned implementation
c) possibility of using large time steps
d) good mass conservation

This article discusses the mathematical model, implementation and numerical validation of a novel two-dimensional Eulerian-Lagrangian embedded formulation applied to PEFC gas channel simulations. Special emphasis is given to the surface tension and contact angle conditions. For the numerical examples solved, the present formulation led to stable and accurate solutions with time steps up to 3 orders of magnitude higher than those obtained with VOF [18]. The model is implemented in two dimensions. A three-dimensional implementation of the model is underway.

The paper is organized as follows. First, the mathematical model is presented, with special attention given to the surface tension term. Next, the contact angle condition is explained, including a dynamic contact angle condition to improve numerical results of droplet deformation on rough surfaces such as GDLs. The model is then compared to sessile and inclined plane experimental results in order to validate the surface tension implementation. Droplet dynamics in a PEFC channel are studied next. A comparison of results with those found using the semi-analytical model presented by the authors in Ref. [7] is also provided. Emphasis is placed on the model capabilities since three-dimensional simulations are required to provide physically accurate results.

2. Numerical model

According to the embedded[1] approach proposed in Refs. [16,17], the two-phase problem is treated in a partitioned manner using the Eulerian and Lagrangian frameworks for air and water, respectively. In this numerical formulation, the Lagrangian sub-domain (water) is moving on top of the fixed Eulerian mesh and the interaction is represented by the boundary condition exchange across the interface. A schematic representation of the embedded air-water setting is shown in Fig. 1. The Lagrangian domain Ω_W is embedded into the Eulerian domain Ω_A. The outer boundary of the Eulerian domain is designated as Γ_A. The boundary of the Lagrangian domain Γ_I defines the position of the interface between both fluids. The intersection between both boundaries is denoted by $\Gamma_S=\Gamma_A\cap\Gamma_I$.

In the following section, the governing equations for both the subdomains and the coupling equations are specified. For further details on the embedded approach for multi-fluids the reader is referred to [17].

2.1. Governing equations

The system considered in the present work is a domain (Ω_A) filled with air and a small fraction of water (Ω_W) within it. In this case, air and water are considered incompressible Newtonian viscous fluids. The governing equations for both fluids are the Navier-Stokes equations (note that it is assumed that gas and liquid are not produced/consumed in the computational domain):

$$\nabla\cdot\mathbf{v} = 0 \text{ on } \Omega_A \text{ and } \Omega_W \tag{1}$$

$$\rho_f\frac{D\mathbf{v}}{Dt} - \nabla\cdot\boldsymbol{\sigma} = \rho_f\mathbf{g} \text{ on } \Omega_A \text{ and } \Omega_W \tag{2}$$

where $\mathbf{v}$ is the velocity vector, $\boldsymbol{\sigma}$ is the Cauchy stress tensor, t is the time, $\mathbf{g}$ is the body force and ρ_f is the fluid density. Since air is modeled using a viscous incompressible fluid formulation and thermal effects are neglected, no equation of state (such as e.g. ideal gas equation) is necessary to close the governing system. For sake of brevity, a single set of equations has been written to represent the governing equations for both fluids. The operator $\frac{D\phi}{Dt}$ stands for the total material derivative:

$$\frac{D\phi}{Dt} = \frac{\partial\phi}{\partial t} + \mathbf{v}\cdot\nabla\phi \tag{3}$$

The convective term $\mathbf{v}\cdot\nabla\phi$ is absent in the Lagrangian formulation.

2.2. Boundary conditions

Boundary conditions for both air and water domain and its interface are imposed in order to solve the problem. A no-slip Dirichlet boundary condition is imposed at Γ_A:

$$\mathbf{v}_A = 0 \text{ at } \Gamma_A \tag{4}$$

Water can have non-zero velocities on the x direction and therefore a slip boundary condition is imposed at Γ_S:

$$\mathbf{v}_W\cdot\mathbf{n} = 0 \text{ at } \Gamma_S \tag{5}$$

At the air-water interface Γ_I, two boundary conditions are

[1] In the CFD community, “embedded” refers to the setting, where a moving mesh is immersed or embedded into a fixed mesh. Alternatively, the term “immersed boundary” method is sometimes used.