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CFD simulation of the two-phase flow for a falling film microreactor

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ABSTRACT

Falling film microreactors, which provide very high specific interfacial area, have become a promising solution to the fast and strongly exothermic/endothermic gas–liquid reaction systems. A computational fluid dynamic simulation of the two-phase flow for a falling film microreactor is presented using the volume of fluid (VOF) model. The hydrodynamic characteristics, from both 2-D and 3-D simulations, including liquid film thickness, velocity, pressure and shear stress profiles, are analyzed. 2-D simulation is adopted for the study of the relationship of liquid flow rate and film thickness, as well as the effects of gas flow rate, surface tension, liquid viscosity and pressure difference on the liquid flow rate. 3-D simulation is necessary to provide the comprehensive flow profiles. Although the system is in the laminar flow regime, the liquid film features a wavy structure and the velocity profiles are complex.

1. Introduction

The advance of microfabrication technology has moved forward the development of various microchemical devices [1], such as mixer, heat exchanger and reactor. For gas–liquid reactions, a falling film microreactor (FFMR) developed by the Institut für Mikrotechnik Mainz GmbH (IMM) can generate stable films less than 100 μm thick [2]. Compared to the 0.5–3 mm film thickness of the conventional falling film reactors, the specific interfacial area can be raised from 100–1000 m^2/m^3 to 5000–50,000 m^2/m^3 [3]. For fast reactions limited by mass and heat transport and/or strongly exothermic or endothermic gas–liquid reactions, FFMRs provide the advantages of high yield, high selectivity, near-isothermal and safe operations.

A comprehensive summary of the studies on FFMR has been given in [4], including studies related to the hydrodynamics, mass and heat transfer, flow equipartition, axial dispersion and demonstration of the performances for various applications [3,5–8]. Most of the investigations were conducted via experimental works. Due to the computational complexity, reported simulation studies were undertaken only for one of the phases and/or with various simplifications on the profiles or interfacial boundary conditions. For example, 2-D and 3-D computational fluid dynamics (CFD) simulations were carried out only for the liquid phase with the simplified assumption of zero interfacial shear force to investigate the concentration dispersion in the liquid phase [9]. In [6], for the CO_2 absorption application, mathematical models were developed individually for gas phase and liquid phase. The models were then related by the interfacial boundary conditions of zero shear stress and phase equilibrium. For the fluorination of toluene process, presuming the mass transfer resistance is in the gas phase, a mathematical model for the gas phase only, which involves the momentum conservation and convective–diffusion equations, was solved to develop correlations for mass transfer coefficient [10]. The gas velocity at gas–liquid interface was set equal to the liquid velocity.

Although the flow is laminar in the micro-channels, due to the small dimensions, the effects of heat conduction, mass diffusion and hydrodynamics, e.g. film thickness, waves and velocity profiles near the gas–liquid interface, on heat and mass transfer become significant. Despite of the computational complexity, it is desirable to implement the two-phase simulation without simplifications to provide a comprehensive picture of the internal profiles of FFMRs.

With the length scale of microreactors, the Knudsen number, which is the ratio of mean free path of the gas molecules and a characteristic length scale of the flow domain, is less than 10^{-2}. The flow regime is continuum flow with no-slip boundary condition and the conventional macroscopic Navier–Stokes equation can be applied [11]. For the laminar two-phase flow in the macro-scale horizontal or vertical tubes, many researchers have found the volume of fluid (VOF) model is suitable for simulating the interface among two or three fluids [3,12–14].

It is essential to investigate the hydrodynamics of the FFMR before the study of the heat and mass transfer rates. This paper presents the 2-D and 3-D CFD simulation of the hydrodynamics for a FFMR using the VOF model. The simulated flow profiles are analyzed. Via the simulation, the effects of fluid properties and flow conditions on the two-phase flow are investigated.

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Nomenclature

$\vec{F}$	external body force per unit volume [N/m^3]
g	gravitational acceleration [m/s^2]
K_F	$\mu^4 g/\rho\sigma^3$
m	mass flow rate [kg/s]
$\hat{n}$	unit vector normal to the liquid film surface
$\hat{n}_w$	unit vector normal to the wall
P	pressure [N/m^2]
Re	Reynolds number
$\hat{t}_w$	unit vector tangential to the wall
$\vec{v}$	velocity vector [m/s]

Greek symbols

α_i	volume fraction of phase i
δ	film thickness [m]
κ	surface curvature [1/m]
μ	viscosity [kg/m s]
ν_L	kinematic viscosity [m^2]
ν'_L	$\nu_L/6\times10^{-7}$
θ	inclination angle from the horizontal
θ_C	contact angle
ρ	density [kg/m^3]
σ	surface tension [N/m]

Subscripts

G	gas
L	liquid

2. Modeling method

The vertical FFMR configuration used in this simulation work is based on the design of IMM [8], as depicted in Fig. 1. The reactor is composed of a reaction plate with multiple open top microchannels, a gas flow chamber and the top/bottom plates. The liquid phase is distributed in the microchannels through a slit and flowing down as a liquid film to a withdrawal zone at the bottom. The width and depth of each microchannel are 300 μm × 100 μm, the depth of gas chamber is 2.5 mm and the gas–liquid contact length is 66.4 mm. For the 3-D and 2-D simulations, the geometries with the inlets and outlets as well as the dimensions are illustrated in Fig. 2. Due to the symmetric nature, only half of a microchannel is simulated in the 3-D study and the symmetric planes are marked with gray color. Also shown in the figures are the horizontal planes and lines, which will be used for simulation results discussion. In the following figures, the axis labeled '*X*', '*Y*' or '*Z*' denotes the *X*-, *Y*- or *Z*-coordinate defined in Fig. 2.

2.1. Governing equations

The commercial CFD code FLUENT 6.3, which is based on the finite volume approach, is used. For the two-phase flow where the two fluids are not interpenetrating, the VOF model can be adopted for tracking the wavy interface. With the VOF model, for each phase, a variable which is the volume fraction of the phase is defined. In each control volume, the volume fractions of all phases sum to unity. The fields for all variables and properties are shared by the phases and represent volume-average values.

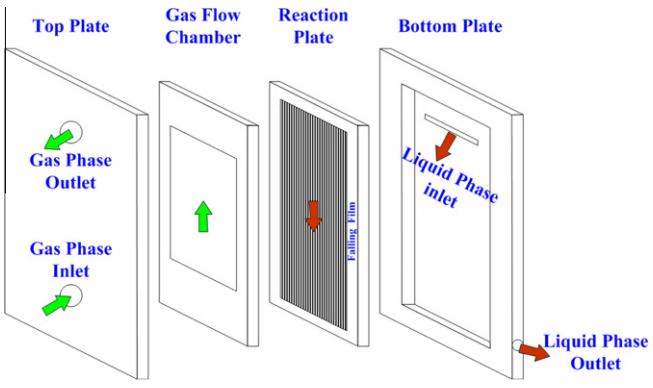

Fig. 1. A falling film microreactor.

The governing equations for the laminar gas–liquid flow include:

$$\text{Continuity for phase } i: \frac{\partial}{\partial t}(\alpha_i\rho_i) + \nabla\cdot(\alpha_i\rho_i\vec{v}_i) = 0 \tag{1}$$

with the constraint of volume fractions as

$$\sum_{i=1}^{n}\alpha_i = 1 \tag{2}$$

$$\text{Momentum}: \frac{\partial}{\partial t}(\rho\vec{v}) + \nabla\cdot(\rho\vec{v}\vec{v}) = -\nabla P + \nabla\cdot[\mu(\nabla\vec{v} + \nabla\vec{v}^T)] + \rho\vec{g} + \vec{F} \tag{3}$$

where the volume-averaged density and viscosity are used. In FLUENT [15], the effect of surface tension along the interface between the phases is included by the continuum surface force (CSF) model [16]. With this model, the addition of surface tension to the VOF calculation results in a source term in the momentum equation. The source term is

$$\vec{F} = \sigma\frac{\rho\kappa\nabla\alpha_i}{\frac{1}{2}(\rho_i+\rho_j)} \tag{4}$$

where κ is the surface curvature and can be computed from local gradients in the surface normal at the interface.

In FLUENT, the effect of the contact angle between the fluid and the wall can be included in the VOF model by the dynamic boundary condition approach. If θ_C is the angle between the wall and fluid, the surface normal of the fluid at the cell next to the wall can be determined by

$$\hat{n} = \hat{n}_w\cos\theta_C + \hat{t}_w\sin\theta_C \tag{5}$$

where $\hat{n}_w$ and $\hat{t}_w$ are the unit vectors normal and tangential to the wall, respectively. The surface curvature determined for the cell can then be used in the surface tension calculation described above.

2.2. Grid system and boundary conditions

Structured grid system with hexahedral or rectangular cells is used for the 3-D and 2-D simulations, respectively. For the zones near inlets, outlets, walls and liquid film, as well as the liquid film, cells with smaller size are employed. Grid independent analysis is undertaken. The analyzed systems using different cell sizes are compared for the ease of convergence and the converged liquid flow rate, the average film thickness, and the wavy characteristics of liquid film. In the *X*- and *Z*-direction, the grid sizes are between