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Direct numerical simulation of interphase mass transfer in gas–liquid multiphase systems ☆

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ABSTRACT

This paper presents the Direct Numerical Simulation of interphase mass transfer in gas liquid multiphase system. The volume-of-fluid (VOF) method in conjunction with mass transfer model has been used. In order to study the process of interphase mass transfer two numerical simulation methods are presented. Two common mass transfer mechanisms, Diffusion through Stagnant Film (DTSF) and Equi-Molal Counter Diffusion (EMCD), are investigated. Two benchmarks, the Stefan diffusion problem and the diffusion in water and methanol Gas–Liquid system, have been used to validate the numerical methods. Afterwards two proposed numerical solution for different mass transfer mechanisms have been investigated in stratified gas liquid flows between two parallel plates. The results show by different approaches in numerical solution, the accuracy of mass transfer simulation is different.

1. Introduction

A group of operations for separating the components of mixtures is based on the transfer of material from one homogenous phase to another. Most of them encounter with gas–liquid two phase mass transfer. Prediction of interfacial mass transfer rate between gas liquid phases plays an important key role in chemical and petrochemical industries. Optimization of mass transfer units requires profound understanding of the principle mass transfer processes. Here, the numerical simulations provide a beneficial tool to reduce the experimental cost for equipment design.

The numerical simulation of interphase mass transfer can be performed by fundamentally two different approaches. The first approach is direct solution of two phase flow and species conservation equations, in which the motion of interface is considered by means of an interface tracking method. The first approach requires adequately fine grids and sufficiently small time steps, and thus, the computational time is very high. Nowadays due to increase in computational power, direct solution of species conservation equations become feasible and prove extremely useful for understanding fundamental phenomena. In the second approach the local equations are not solved and the averaged governing equations are used instead. This approach needs empirical correlations for computing the gas–liquid interphase mass transfer coefficient. The generality of this approach is limited since it always relies on certain assumptions for mass transfer and thus requires appropriate closure models.

In the direct approach the two phase flow field which is needed for calculation of convective mass transfer, is obtained by solving the Navier–Stocks equations. There are different interface tracking methods for simulation of multiphase flow like VOF [1], level set [2] and front tracking [3]. Among these approaches, the VOF method, fixed grid technique for two or more immiscible fluids, is one of the most widely used methods.

The first simulation for interphase mass transfer with the VOF method was reported by Ohta and Suzuki [4]. They studied mass transfer from a rising drop in a solvent extraction process. Coupling of VOF method with mass transfer was also depicted by Davidson and Rudman [5]. They calculated the mass transfer from a rising drop through a liquid column. Schlottke et al. [6], Onea et al. [7] and Bothe et al. [8] used the VOF method for direct numerical simulation of interphase mass transfer. Petera and Weatherley [9] investigated the mass transfer from a falling axsymmetric drop using a finite element method. This method was also used by Waheed et al. [10] to compute the mass transfer of single spherical drops by free and forced convection. Comprehensive two-dimensional investigations of the liquid-sided mass transfer from single bubbles and bubbles swarms with constant concentration in the bubbles have been performed using a front-tracking method [11,12]. Haelssig et al. presented a VOF methodology for direct numerical simulation of interface dynamics and simultaneous interphase heat and mass transfer in systems with multiple chemical species [13]. The VOF method was also used to study the transport phenomena encountered in developing falling film evaporation [14], volatile liquid evaporation from capillary tube [15], nucleate boiling [16], fuel tank splash loading [17], solidification shrinkage [18] and droplets impingement onto a substrate [19].

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Nomenclature

A	Area
D	Diffusion coefficient
g	Gravity acceleration
l	Film thickness
M	Molecular weight
n	Mass flux
p	Pressure
R	Gas constant
S	Source term
t	Time
T	Temperature
u	Velocity
$\overline{u}$	Diffusion velocity
x	Mole fraction
Z	Compressibility factor

Greeks

α	Volume fraction
ν	Kinematic viscosity
μ	Dynamic viscosity
ρ	Density
ω	Mass fraction

Subscripts

b	Bulk
eq	Equilibrium
g	Gas
i	ith component
j	jth component
l	Liquid
v	vapor

In the absence of chemical reaction, there are two mechanisms which frequently arise in gas liquid multiphase systems [20]: Diffusion through Stagnant Film (DTSF) and Equi-Molal Counter Diffusion (EMCD).One important issue in the Direct Numerical Simulation of different interphase mass transfer mechanisms is the effect of mass transfer on hydrodynamics of system. DTSF mechanism is very common in many chemical engineering processes, in which one component has zero flux such as condensation, evaporation and absorption. In this mechanism, system hydrodynamics is affected by interphase mass transfer and this effect generate the diffusion velocity at interface. EMCD is a situation which frequently pertains in distillation operations. In EMCD mechanism, any molecules movement of a species in a direction must be balanced by a movement of the molecules of other species in the opposite direction, so in this mechanism mass transfer has no effect on system hydrodynamics. The mass transfer effect on system hydrodynamics is of essential importance and this effect determine the nature of mass transfer process between two phases. Van Baten and Krishna [21] studied the DTSF mass transfer from Taylor bubble rising in circular capillaries. They ignored the effect of mass transfer on the hydrodynamic behavior of the system. They also studied the DTSF interphase mass transfer and reaction in another work [22], but again the effect of mass transfer on two phase flow hydrodynamics has been neglected. Ambrosini et al. [23] studied the DTSF process of evaporative cooling by computational fluid dynamics, in which they neglected the effect of mass transfer on the system hydrodynamics. Moreover, they assumed that the liquid film thickness was very thin and the liquid film effect is negligible in mathematical modeling [23]. Banerjee used the VOF method to study of heat and mass transfer in stratified flow through the automotive filler pipe [24,25]. In these studies, the effect of mass transfer on the hydrodynamics of the system was considered; whereas the fuel evaporation is one-way diffusion (DTSF approach) but they implemented the source terms in the transport equations based on Equi-Molal Counter Diffusion (EMCD). In most of the previous studies the hydrodynamics effect of mass transfer on mass transfer mechanisms was neglected.

This article presents the Direct Numerical Simulation of the different interphase mass transfer mechanisms in the gas–liquid multiphase systems. To this aim, two numerical methods have been investigated with the purpose of numerical studying the DTSF and EMCD mass transfer mechanisms. These numerical methods were used to simulate the two-dimensional Stefan problem and mass transfer in gas liquid stratified flow between two parallel plates.

2. Mathematical modeling

2.1. Diffusion through Stagnant Film (DTSF)

In order to study the DTSF interphase mass transfer mechanism, two numerical methods have been investigated. In the first method, the effect of mass transfer on system hydrodynamics is considered directly by applying the source term to continuity/species equations. In another method, mass transfer influence on system hydrodynamic is taken into account indirectly by implementing some modification on the species conservation equations.

2.1.1. Source term for gas continuity equation

In this approach, it's named “First Method”, for numerical simulation of interphase mass transfer with DTSF mechanism, continuity, momentum and conservation equation of transport component are solved. The VOF model enables the interface tracking for gas–liquid multiphase flows. In the VOF model, the variables such as pressure and velocity are shared by both phases and correspond to volume-averaged values. The volume-averaged conservation equations for mass and momentum describing the flow of two immiscible fluids are expressed as follow, respectively:

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho u) = 0 \tag{1}$$

$$\frac{D\rho u}{Dt} = -\nabla p + \mu\nabla^2 u + \rho g \tag{2}$$

Mixture density and dynamic viscosity are determined by volume fraction averaging.

$$\rho = \alpha\,\rho_v + (1-\alpha)\,\rho_l \quad \mu = \alpha\,\mu_v + (1-\alpha)\,\mu_l \tag{3}$$

Continuity equation for the gas phase volume fraction, α, is:

$$\frac{\partial \rho_V \alpha}{\partial t} + \nabla\cdot(u\,\rho_V\,\alpha) = S_i \tag{4}$$

Where mass transfer rate per unit volume of transport component is given by:

$$S_i = \frac{D_{ij}\,\rho_V}{1-\omega_i}\nabla\omega_i\,|_{\text{interface}}\cdot A \tag{5}$$

This mass transfer rate is calculated only into cells which the gas volume fraction is not equal to zero or one ($0<\alpha<1$). In Eq. (5), **A** is the normal interfacial mass transfer area is given by,

$$A = V_{\text{cell}}\nabla\alpha \tag{6}$$