Chemical Engineering Science 138 (2015) 741–759

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

A computational study of the interfacial heat or mass transfer in spherical and deformed fluid particles flowing at moderate Re numbers

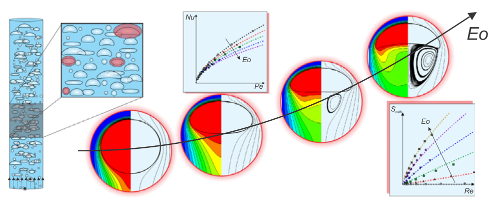
R.F.L. Cerqueira, E.E. Paladino*, C.R. Maliska

SINMEC - Computational Fluid Dynamics Lab, Mechanical Engineering Department, Federal University of Santa Catarina, 88040-900 Florianopolis, SC, Brazil

HIGHLIGHTS

- The interfacial heat transfer around spherical and distorted fluid particles is studied.
- A correlation for Nusselt number in deformed fluid particles is proposed.
- The distortion also affects the interfacial area density.
- A correlation for the interfacial area correction is also proposed.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 11 March 2015
Received in revised form
28 August 2015
Accepted 31 August 2015
Available online 18 September 2015

Keywords:
Interfacial heat transfer
Distorted fluid particles
Volume-of-Fluid
Two-Fluid model closure

ABSTRACT

In this paper, the interfacial heat transfer in spherical and distorted fluid particles, flowing at *Re* numbers up to 80.0, is studied through the Volume-of-Fluid approach, aiming the development of closure relations for the interfacial heat and mass transfer, in the context of the Two-Fluid model. The Nusselt numbers of spherical particles are compared with the usual correlations presented in the literature to validate the numerical model. From the approach adopted in this work, based on the detailed modeling of the interfacial heat transfer process, it is possible to analyze the local flow structure and thermal field around the fluid particles, providing a better understanding of the effect of the particle deformation on the global heat transfer coefficients. It is shown that the interfacial heat flux distribution is affected by the particles shape, which substantially affects the flow and thermal fields around the fluid particles and, consequently, the total heat transfer rate. In addition, the effect of the increase of the interfacial area density, due to the particle deformation, on the total interfacial heat transfer is analysed. New correlations are proposed for the interfacial *Nu* or *Sh* numbers, in single rising fluid particles, which become dependent on the Eötvös (*Eo*) number, and for the correction of the interfacial area density, which should be included in the closure of the interfacial heat or mass transfer terms in the Two-Fluid model equations. It is shown that, as the particles become distorted, the transfer coefficient decreases, but the interfacial area increases, compensating the effect on the total interfacial flow. Nonetheless, for highly distorted particles, the effect of the interfacial area increase becomes dominant and the resulting total interfacial transfer is higher than the case of spherical particles.

1. Introduction

Gas–liquid two-phase flows are frequently encountered in the oil, chemical and energy transformation industries. Some specific applications in oil and gas industry related to flow assurance problems, such as wax deposition, hydrate formation and corrosion problems by CO_2 and H_2S among others, require, in addition

* Corresponding author.
E-mail addresses: rafaelfc@sinmec.ufsc.br (R.F.L. Cerqueira), paladino@sinmec.ufsc.br (E.E. Paladino), maliska@sinmec.ufsc.br (C.R. Maliska).

http://dx.doi.org/10.1016/j.ces.2015.08.054
0009-2509/

to the interfacial momentum transfer, the detailed modeling of the heat and mass transfer processes between phases. In the chemical and petrochemical industries, the need of these detailed models is necessary in the refining processes, design of distillation columns and bubble column reactors, as shown, for instance in the works of Krishna and van Baten (2002, 2003), Kantarci et al. (2005), and Singh and Majumder (2011).

Bubbles of different sizes and shapes are encountered in several flow patterns, ranging from spherical ones in finely dispersed bubbly flow to Taylor bubbles in slug flow. Even in slug flow pattern, small dispersed bubbles flow within the liquid slugs between two consecutive Taylor bubbles. The simulation of these flows requires precise closure models for interfacial transfer, even in one-dimensional approaches, utilized in flow in wells, or multi-dimensional models employed in the modeling of the flow inside pumps, separators and other primary oil treatment as well as distillation columns or bubble column reactors.

For the case of interfacial momentum transfer, several closure relations have been presented in the literature (Ishii and Hibiki, 2011; Clift et al., 1978) including correlations for the cases of distorted (non-spherical) bubbles or droplets as the classical Ishii–Zuber (Ishii and Zuber, 1979) or Grace (Clift et al., 1978) correlations. On the other hand, in modeling interfacial heat and mass transfer processes, in the context of the Two-Fluid model for dispersed flow patterns the usual practice is to employ classical correlations based on *Re* and *Pr* or *Sc* dimensionless groups, but considering perfectly spherical shaped bubbles (Ranz and Marshall, 1952; Lochiel and Calderbank, 1964; LeClair and Hamielec, 1971; Oellrich et al., 1973; Takemura and Yabe, 1998), which can lead to significant discrepancies in the calculation of the total interfacial heat or mass transfer. In a general way, the heat and mass transfer between phases in bubbly flow regime is still not fully understood and is a topic of ongoing research (Hayashi et al., 2014; Bothe and Fleckenstein, 2013; Aboulhasanzadeh et al., 2012, 2013; Marschall et al., 2012).

One of the main difficulties in modeling multiphase, multi-component and non-isothermal flows is the interface tracking and its definition, as well as the transfer mechanism and calculation between the two (or more) distinguished domains.

Most of the recent numerical works exploring the interfacial heat and mass transfer utilize interface capturing methodologies, based on the solution of a transport equation in an Eulerian frame, to implicitly define the interface position, such as Volume-of-Fluid (Bothe and Fleckenstein, 2013; Marschall et al., 2012) or Level-Set (Yang and Mao, 2002, 2005) or Front-Tracking methods based on the lagrangian tracking of the interface position (Aboulhasanzadeh et al., 2012, 2013; Wang et al., 2008).

For the inclusion of the interfacial heat and mass transfer phenomena into the models, some approaches have been proposed in the literature. In the recent paper of Marschall et al. (2012), the authors propose a new method for the calculation of the interfacial mass transfer fluxes, called the Continuous-Species-Transfer (CST) which is based on an analogy of the well-known Continuous-Surface-Force (CSF) method (Brackbill et al., 1992). Through this approach, the authors were able to model the interfacial jump in the concentration field, which arises for equilibrium coefficients different from one, in the context of the VOF model. Another alternative to calculate the interfacial mass and heat transfer is to utilize the overall energy or mass balance concept, as shown in Hase and Weigand (2004) and Wang et al. (2008). Recently, some authors also proposed the use of subgrid-scale methods (Aboulhasanzadeh et al., 2012, 2013; Bothe and Fleckenstein, 2013; Hayashi et al., 2014), which, in general, are based on the use of known solutions, based on boundary layer theory, to predict the interfacial transfer in the near interfacial regions, to save computational effort, mainly in cases of high Schmidt *Sc* or Prandtl *Pr* number, where the thermal or concentration boundary layer at the interface becomes very difficult to be resolved with practicable mesh sizes. Hayashi et al. (2014) and Aboulhasanzadeh et al. (2013) showed that the subgrid-scale approach presents good agreement when compared to experimental results, in spite of its various assumptions.

Another alternative in modeling interfacial heat transfer is to employ body fitted grids with increased resolution near the fluid particle surface. Figueroa-Espinoza and Legendre (2010) studied the mass transfer of a spheroidal bubble rising through a stationary liquid for various flow and geometrical configurations, analysing the local and global mass transfer. The main disadvantage of such an approach is the fact that the interface morphology is imposed, while, in reality, it results from the balance between the inertial, viscous and surface tension forces, not allowing us to link the obtained results with the adequate dimensionless parameters that describe the phenomena, such as Eötvös or Weber numbers. In addition, some hypothesis regarding the flow behavior at the interface, which, in this approach corresponds to a domain boundary, must be assumed. In general, free slip or no-slip conditions are assumed, for high and low viscosity relations, but this is not consistent in several cases. An important remark of the work of Figueroa-Espinoza and Legendre (2010) is the discussion about the need of correction factors in the average heat or mass transfer coefficient and in the interfacial area, to consider the effects of the deviations from a spherical shape, in the application of mass transfer correlations in the Two-Fluid Model.

Although some works investigate the effect of particle distortion on the interfacial heat and mass transfer, some of them through very sophisticated models, no works have been encountered presenting a systematic analysis aiming to develop closure relations for the application within the Two-Fluid Model.

The approach used here takes into account the internal flow within the particle on the flow structure around it and, beyond the restrictions of moderate Reynold and Prandtl numbers (*Re* up to 100 and *Pr* up to 10) imposed by the modeling approach employed, no other assumptions such as sub-grid known solutions, potential flow or asymptomatic limits for *Pr* (or *Sc*) number have been imposed. In addition, considering the reference frame attached to the fluid particles, by using a proper coordinate transformation, and keeping the temperature of the fluid particle constant along the simulation, by adding a suitable source term into the energy equation, allowed for very long term simulations which guaranteed the full development of hydrodynamic and thermal fields around the fluid particles for all ranges of *Re* and *Pr* numbers considered.

In this way, a systematic study was performed, varying the non-dimensional parameters which govern the interfacial heat transfer to determine, through a detailed modeling of the flow around fluid particles with different interface shapes, the interfacial heat and mass transfer coefficients. Through this study, it was possible to advance in the comprehension of how the interface shape affects the process and, ultimately, the global heat and mass transfer coefficients, which are needed for the Two-Fluid Model closure. From the data fitting of global transfer coefficients obtained from simulations, correlations are proposed which should improve the predictions of interfacial transfer with the Two-Fluid Model.

2. Methodology

In order to study the effect of the fluid particle shape and its implications on the interfacial heat transfer, several cases were simulated for different values *Eo* and *Re* numbers. This was accomplished by simulating a rising bubble, where the fluid