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A CFD model for the coupling of multiphase, multicomponent and mass transfer physics for micro-scale simulations

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ABSTRACT

This paper presents a CFD model that couples the physics of multiphase and multicomponent flow involving mass transfer for micro-scale simulations. The volume-of-fluid (VOF) model is utilised to capture the multiphase physics, and smoothing operations are applied in the surface tension force calculation to minimise spurious velocities. For multicomponent tracking of the species transport, the α-factor and expulsion operation methods are implemented to ensure that the species are tracked within the correct phase. Three different mass transfer models were adopted with modifications to the original models. The developed coupled multiphase-multicomponent model was assessed via a series of validation cases: a simple one-dimensional (1D) diffusion problem, horizontal vapour flow over a smooth stationary liquid where Sherwood number was used to measure mass transfer performance, and the dissolution of a two-dimensional (2D) droplet. In all the test cases, the model was able to yield reasonably close results with the analytical solution or empirical correlations used in the validation, thus establishing its accuracy and reliability of the developed model. Simulations using the coupled multiphase-multicomponent model represent a cost-effective approach to obtaining insights into the flow physics for a variety of applications: dissolution of droplets in microchannels, transport of drugs in blood vessels that entails mass transfer and simulations of carbon dioxide enhanced oil recovery at the pore-scale.

1. Introduction

Many processes and applications in the industry involve fluid systems that encompass various complex flow physics: different phases co-existing, mass transfer and multiple chemical species. These systems prevail across various scales, from large-scale bubble column reactors used in chemical, petrochemical, biochemical and metallurgical industries [1] to the micro-scale transport of droplets in microchannels for drug delivery applications [2]. Numerical simulations can provide effective means of studying the flow behaviour and obtaining crucial insights into the design of such devices. However this can only be made possible if the numerical model used is able to capture all the complex flow physics aforementioned.

Much advancement has been made in the development of multiphase computational methodologies: level-set method [3,4], front-tracking method [5] and the Shan-Chen model for multiphase modelling using the lattice Boltzmann method [6,7]. These models have subsequently been used to investigate problems involving mass transfer. Yang and Mao [8] adopted the level-set approach to simulate interphase mass transfer and validated their model using experimental results of a rising deformable droplet. Koynov et al. [9] applied the front-tracking method to investigate the mass transfer and flow dynamics of bubble swarms in order to study their impact on chemical reactions.

The most widely used interface capturing model is he volume-of-fluid (VOF) method which was first developed by Hirts and Nichols [10]. The model utilises a VOF function α to track the volume fraction of the different phases, and a Piecewise-Linear Interface Calculation (PLIC) method [11,12] to approximate the multiphase interface. Many authors have successfully implemented mass transfer models for multiphase systems that accommodate the VOF model as the base model [13–15]. Furthermore, the VOF model has also been used to investigate simultaneous heat and mass transfer for a variety of problems, including bubble growth during boiling in a microchannel [16,17], heat and mass transfer in an inclined channel [18], nucleate boiling in microchannels [19,20] and evaporation [21]. In these numerical models, the issue of spurious velocities persists which are the non-physical velocities that arise due to discretisation errors in the surface tension force calculation. This problem is exacerbated at the

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micro-scale as capillary forces dominate, which may compromise the accuracy of simulations at the micro-scale. Recently, innovative approaches have been developed to minimise the issue of spurious velocities in the VOF model [22–25] and have been successfully used to investigate micro-scale problems involving pore-scale [26,27] and microchannel [28] flows.

In addition, the VOF model has also been adopted to simulate the physics of multiphase flow with multicomponent species tracking in the presence of mass transfer simultaneously. Bothe and Fleckenstein [29] implemented a mass transfer model that is calculated based on the product of the diffusion coefficient and species concentration gradient. The model was assessed for the simulation of oxygen transfer from rising three-dimensional (3D) bubbles and obtained good agreement with experimental data. Haelssig et al. [30] developed a model that computes the mass transfer rate based on the conservation of species from the interface jump in the presence of heat transfer, and validated their results with empirical Sherwood number correlations. Other models have also been proposed that account for the discontinuity in species concentration across the multiphase interface [31–34]. The practicality of these models have been demonstrated through their usage in studying a variety of applications, including the dissolution of CO_2 droplets in methanol and ethanol in a microchannel [35], a membrane separation process [36] and determining the mass transfer and liquid hold-up in structured packing [37].

Much development have been performed on the interface capturing models based on VOF coupled with the tracking of multicomponent species, as evidenced by the aforementioned literature. Nonetheless, many of these models fail to address the issue of spurious velocities which will encumber the reliability of results for multiphase-multicomponent simulations at the micro-scale. Furthermore, most models employ a single species transport equation to track the flow of a species type in all phases. This is useful in providing the overall flow behaviour of the species but may prove difficult when the behaviour of the species in a specific phase are required to be locally predicted. For instance, for the problem of a dissolving CO_2 droplet within silicone oil flowing in a microchannel, one might be interested in studying the flow physics of the dissolved CO_2 within the silicone oil, and in this case having a species transport equation that solves specifically for the transport of dissolved CO_2 within silicone oil will be more relevant.

In this paper, a coupled multiphase-multicomponent model that is applicable for micro-scale problems is presented. In the next section, the development of the model with all the required physics is described in detail: multiphase governing equations, method to minimise spurious velocities, mass transfer and calculation of interfacial area, multicomponent and tracking of species within the correct phase. In Section 3, three validation cases are employed to test the accuracy and reliability of the coupled multiphase-multicomponent model.

2. Mathematical and numerical formulation

2.1. CFD governing equations and multiphase modelling

The coupled model developed in this work requires the simultaneous simulation of both multiphase and multicomponent physics. For the multiphase modelling, we adopt the *interFoam* volume-of-fluid (VOF) solver in OpenFOAM 2.3. The VOF multiphase model was first proposed by Hirts and Nichols [10] and uses a VOF function α to track the volume fraction occupied by each phase in the individual mesh cells. The model is assumed to be Newtonian, incompressible and isothermal. The isothermal assumption is valid for dissolution mass transfer with minimal temperature variation (e.g. dissolution of CO_2 in silicone oil). The density ρ and viscosity μ are calculated via the α-weighted average of the phases occupying each cell:

$$\rho = \alpha_1\rho_1 + \alpha_2\rho_2 \tag{1}$$

$$\mu = \alpha_1\mu_1 + \alpha_2\mu_2 \tag{2}$$

where the subscripts 1 and 2 refer to the different phases under consideration, with $\alpha_1 = \alpha$ and $\alpha_2 = 1 - \alpha$. When mass transfer is included, a source term is added to the right hand side of the α-transport equation:

$$\frac{\partial\alpha}{\partial t} + \nabla\cdot(\alpha\mathbf{V}) = \frac{1}{\rho_1}Ja_{VOF} \tag{3}$$

where $\mathbf{V}$ is the velocity vector, J is the mass transfer flux rate coefficient (to be discussed in Section 2.5) and a_{VOF} is the interfacial area density, which will be further elaborated in Section 2.4. The α-transport equation is then solved together with the continuity and momentum equations to fully define the flow field:

$$\nabla\cdot\mathbf{V} = \left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right)Ja_{VOF} \tag{4}$$

$$\frac{\partial\rho\mathbf{V}}{\partial t} + \nabla(\rho\mathbf{V}\cdot\mathbf{V}) = -\nabla p + \rho\mathbf{g} + \nabla\cdot\mu(\nabla\mathbf{V} + \nabla\mathbf{V}^{\mathrm{T}}) + \mathbf{F}_\sigma \tag{5}$$

where p, $\mathbf{g}$, and $\mathbf{F_\sigma}$ are the pressure, gravity, and surface tension force, respectively. The right hand side term in Eq. (4) accounts for the fluid expansion/contraction due to the mass transfer whilst maintaining mass conservation. The surface tension force $\mathbf{F_\sigma}$ is modelled using Brackbill's [38] model of the Continuum Surface Force (CSF):

$$\mathbf{F}_\sigma = \sigma k\mathbf{n} \tag{6}$$

In Eq. (6), σ is the interfacial tension, $\mathbf{n} = \nabla\alpha/|\nabla\alpha|$ is the interface normal which is non-zero only at the interface, and $k = \nabla\cdot\mathbf{n}$ is the interface curvature. From a physical point of view, the expression for curvature k captures the degree of change in the interface normal vector $\mathbf{n}$ along the surface of the multiphase interface, which describes how curved the interface is (e.g. a sharp change in normal vector $\mathbf{n}$ over a short distance implies that the interface is highly curved).

2.2. Smoothing operations to alleviate spurious velocities in multiphase modelling

Although the VOF model is able to simulate multiphase problems requiring the tracking of the interface, nevertheless as with all multiphase numerical models it suffers from the issue of spurious velocities or parasitic currents. These are non-physical velocities that arise due to the numerical errors from the discretisation of the interface curvature, which is used to calculate the surface tension force [39]. This error in the surface tension then propagates into the momentum equation and necessitates the velocity terms to balance them, resulting in the spurious velocities. The problem is exacerbated at the micro-scale where capillary forces dominate [24] and must therefore be addressed to simulate accurate flow behaviour at the micro-scale.

To minimise the spurious velocities, we adopt a series of smoothing operations when computing the interface curvature. Firstly, the α-field is smoothed using a recursive interpolation between the cell and face centres for each grid cell [22,23]. The smoothing operation works by interpolating the cell centre α-values into the face centre values, and then interpolating from the new face centre values back into the cell centre values, recursively. This smoothing operation is applied twice to the α-field: