Chemical Engineering Science 101 (2013) 165–174

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Science

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

# A validation of an embedded analytical description approach for the computations of high Schmidt number mass transfer from bubbles in liquids

B. Aboulhasanzadeh [a,*], S. Hosoda [b], A. Tomiyama [b], G. Tryggvason [a]

[a] University of Notre Dame, Notre Dame, IN 46556, USA
[b] Kobe University, 1-1 Rokkodai, Nada, Kobe 657-8501, Japan

## HIGHLIGHTS

- Mass transfer in high Schmidt number bubbly flows is found using a multiscale method.
- A boundary layer model is used for the mass transfer next to the bubbles.
- A finite volume method is used for the mass transfer in the rest of the flow.
- A comparison with experimental results and correlations shows good agreement.
- Using this multiscale approach results in significant reduction in computational cost.

## ARTICLE INFO

*Article history:*
Received 23 January 2013
Received in revised form
13 May 2013
Accepted 7 June 2013
Available online 15 June 2013

*Keywords:*
Bubble columns
Computation
Mass transfer
Multiscale
Transport processes

## ABSTRACT

A multiscale approach for simulations of high Schmidt number mass transfer from bubbles into liquids is validated by detailed comparisons with experimental results. The approach is based on an embedded analytical description of the mass boundary layer next to the bubbles surface, coupled with a finite volume method for the rest of the domain. Two classes of bubbles are examined: Taylor bubbles in a pipe and freely rising bubbles. For the first class an axisymmetric domain is used, while for the latter a fully three-dimensional domain is used to capture the unsteady manner of a rising bubble. We also perform calculations of non-deformable freely rising bubbles for which we compare the computational results with analytical and semi-empirical correlations as well as experimental results from other authors. Mass transfer computations using the embedded analytical description approach show good agreement with the experimental results and the correlations. Based on the ratio of the thickness of the mass boundary layer to the grid size used to resolve the fluid flow we estimate that the use of the presented approach reduces the computational cost at least by one or two orders of magnitude, specially when applied in simulations of fully three-dimensional flows.



## 1. Introduction

One of the most important applications of bubbly flows is in bubble columns (Deckwer, 1992; Furusaki et al., 2001). Their structure and operations are simple, but predicting their performance can be difficult. Computational models cannot at the present time resolve the complete flow field fully and it is therefore necessary to rely on subgrid models for unresolved scales. Such models have traditionally been constructed by scaling analysis and experimental correlations, but as Direct Numerical Simulations (DNS) of the motion of a large number of bubbles in turbulent flows become more commonplace (Bolotnov et al., 2011; Esmaeeli and Tryggvason, 2005; Lu et al., 2005; Lu and Tryggvason, 2007, 2008; Tryggvason et al., 2011), more accurate and universal closure models are likely to be developed. However, the final outcome of a computational model of a bubble column is mass transfer and chemical reactions, not just the fluid flow and the bubble motion. Subgrid models are therefore also needed for those processes. DNS of mass transfer are, so far, very limited and fully resolved results are only available for single bubble or two-dimensional flows. The reason is that mass transfer in liquids is much slower than the momentum transfer so that a mass boundary layer near the surface of the bubbles is much thinner than the momentum boundary layer and the resolution requirement of DNS is set by the number of grid points needed to resolve

* Corresponding author. Tel.: +1 574 631 7148.
*E-mail addresses:* aboulhasanzadeh.1@nd.edu, bahman.ab@gmail.com (B. Aboulhasanzadeh).

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http://dx.doi.org/10.1016/j.ces.2013.06.020

the mass transfer rather than the fluid flow. This can increase the number of grid points needed for a given problem by a factor of a hundred to a thousand or more. For a single bubble several authors have computed the mass transfer, either using body fitted grids where the grid points can be concentrated near the bubble surface (Figueroa-Espinoza and Legendre, 2010; Jung and Sato, 2005; Mao et al., 2001; Ponoth and McLaughlin, 2000) or using regular fixed grids (Hassanvand and Hashemabadi, 2012; Hayashi and Tomiyama, 2011; Onea et al., 2009; Wang et al., 2008). Computations with multiple two-dimensional bubbles and reaction (Koynov et al., 2005; Radl et al., 2008) have been done by using finer grid for the mass conservation equations than the fluid flow equations, but doing so increases the cost significantly, particularly for fully three-dimensional systems.

In the absence of reactions, the mass transfer is a relatively simple problem, except for the disparity in scale with the fluid flow. It is well described by a single scalar advection–diffusion equation and for simple velocity fields the mass distribution will generally exhibit a simple structure. In Aboulhasanzadeh et al. (2012) we introduced a multiscale strategy where we use an embedded analytical description to follow the evolution of the mass distribution near the bubble surface and a regular conservative finite volume method for the evolution away from the bubble. The method is based on a simple boundary layer description of the mass transfer near the surface and was shown to capture both the structure of the mass distribution and the transfer of mass from the bubble to the liquid very well. The accuracy was established by comparing results using this method with simulations where the mass transfer was computed using grids that were sufficiently fine so the mass transfer was accurately resolved. This approach did, however, restrict the comparison to moderate Schmidt numbers ($O(10)$) and two-dimensional flows. Subscale models to fill the gaps between the length and time scales of fluid flow and mass have also been presented by Booty and Siegel (2010) and Bothe et al. (2011).

Here we continue to test the accuracy of this approach by conducting detailed comparisons with experimental results specifically designed to validate the method for high Schmidt number, $Sc = 8260$, and high Reynolds number, $Re \cong 350$. We use an axisymmetric code for simulating Taylor bubbles in a narrow pipe and a 3D code for simulations where axisymmetry is not a feasible assumption. Additionally, we compare the results for freely moving non-deformable bubbles with analytical, semi-empirical correlations and experiments from other authors for Reynolds number ranging from 20 to 110 with $Sc = 100$ and 1000.

## 2. Computational approach and multiscale model

### 2.1. Numerical method

Direct Numerical Simulations of multi-bubble systems are almost exclusively done using the one-fluid form of the Navier–Stokes equations. In this approach, one set of governing equations is solved everywhere, using a regular structured grid, but the material properties, density and viscosity, are set based on an indicator function that marks the different fluids and is advected by the flow. The fluid equations are generally integrated in time using a projection method and a finite volume or finite difference approximations for the spatial derivatives. The indicator function can be advected using several different techniques, such as the volume of fluid (VOF) or level set methods, but here we use the front tracking method originally introduced by Unverdi and Tryggvason (1992), where the boundary between the different fluids is marked by connected marker particles moving with the flow. The indicator function is then constructed from the location of the marker points. The markers are also used to find the surface tension. For a more detailed description of the method, see Tryggvason et al. (2001, 2011), and for its use for DNS of bubbly flows see Bunner and Tryggvason (2002a, 2002b, 2003), and Lu and Tryggvason (2008), for example.

### 2.2. Multiscale model

The primary difficulty in numerical simulations of mass transfer from bubbles in most liquids is the slow diffusion of mass, compared with the diffusion of momentum, which results in a mass boundary layer that is thin compared to the momentum boundary layer at the bubble surface. However, since the mass transfer from the bubbles is proportional to the normal gradient of the concentration of dissolved mass, the boundary layer must be resolved sufficiently well so that the gradient can be computed accurately. A brute force approach would require a very fine resolution that is generally impractical if the intend is to follow the motion of many bubbles. The boundary layer does, however, have a very simple structure and in Aboulhasanzadeh et al. (2012) we showed that its evolution can be accurately captured by a boundary layer description where a parabolized advection–diffusion equation is solved by a simple integral method. Thus, we solve the advection–diffusion equation for the evolution of the mass concentration $f$ by splitting it up into two parts. Away from the bubble surface we solve

$$\frac{\partial f}{\partial t} + \nabla \cdot (\mathbf{u} f) = D \nabla^2 f \tag{1}$$

with an additional sink term, as discussed in Aboulhasanzadeh et al. (2012), using a conservative finite volume scheme. Close to the interface we solve a parabolized version of Eq. (1) which provides a source term when the boundary layer grows over a certain limit. Here, we compare the results from the model with experimental results for two different types of bubbles, Taylor bubbles and oscillating three-dimensional bubbles. For the Taylor bubbles we use an axisymmetric code to compute the bubble dynamics in a cylinder, while for the oscillating bubbles, where the axisymmetric assumption is not feasible, we use a version of the code written for fully three-dimensional domains. In the following subsection the multiscale model is explained first for the axisymmetric and then for the three-dimensional simulation.

#### 2.2.1. Axisymmetric model

For the boundary layer in the case of axisymmetric flow we define the zeroth-moment of the mass concentration by

$$M_0^{ax} = \int_0^{\delta_0} rf \, dn \tag{2}$$

here $n$ is the coordinate normal to the bubble surface, $r$ is the radial distance from the axis of symmetry, and the upper bound $\delta_0$ is the boundary layer limit selected so that it is generally larger than the thickness of the boundary layer $\delta$.

To extract the boundary layer equation we write Eq. (1) in a control volume form for a small segment of the mass boundary layer as shown in Fig. 1:

$$\begin{aligned} \frac{\partial}{\partial t}(rf \, dn \, ds) - u_n rf \, ds + \left(u_n rf + \frac{\partial (u_n rf)}{\partial n} \, dn\right) ds \\ - u_s rf \, dn + \left(u_s rf + \frac{\partial (u_s rf)}{\partial s} \, ds\right) dn \\ = -D\left(r \frac{\partial f}{\partial n}\right)_{n=0} ds + D\left(r \frac{\partial f}{\partial n}\right)_{n=dn} ds, \end{aligned} \tag{3}$$

in which we have neglected diffusion terms in the tangential direction as well as all curvature effects. Assuming $\alpha$ to be a Lagrangian marker (and a constant at each front marker point),