Chemical Engineering Science 176 (2018) 609–621

Contents lists available at ScienceDirect

Chemical Engineering Science

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

Simulations of droplet merging with free surface and bubble column reactor with Finite-size Lagrangian particle tracking

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HIGHLIGHTS

- A criterion is derived to simulate droplets and bubbles merging with free surface.
- Finite-size Lagrangian particle tracking is extended to handle bubbles collisions.
- Bubble column reactor is simulated with Finite-size Lagrangian particle tracking.
- Very good agreement is obtained for the time-averaged liquid velocity profile.

ARTICLE INFO

Article history:
Received 4 September 2017
Received in revised form 19 October 2017
Accepted 23 October 2017
Available online 10 November 2017

Keywords:
Dispersed flows
Finite-size Lagrangian particle tracking
Bubble column reactor
Two-way coupling

ABSTRACT

In this work, we present the latest developments in the finite-size Lagrangian (FSL) tracking method we have recently proposed (Badreddine et al., 2015). The FSL method covers the situations in which dispersed-phase interfaces (bubbles or droplets) are larger than individual computational cells used in simulation, and thus not amenable by Lagrangian particle tracking (LPT). But in the same time, these interfaces are not large enough to be accurately simulated with interface tracking (IT) methods for a given mesh. The FSL method thus covers the middle ground between LPT and IT methods. It also inherits properties of the two; bubbles' shapes and sizes are prescribed with a phase indicator function and the continuous phase is resolved in Eulerian single-fluid framework as it would be in an IT method, and yet, the forces on individual bubbles are corrected from hydrodynamic force correlations used in LPT methods. After the initial phase of the FSL method verification, which was mainly focused on simulations of single moving bubbles, we now apply it to the real case of a square bubble column reactor, and compare time-averaged and fluctuation liquid velocity profiles against experiments. The distinct advantage of the FSL method, over the standard LPT, is the explicit resolution of turbulent structures, including the wakes behind individual bubbles. Bubble plume meandering was captured well in the simulations, as well as time-averaged vertical velocities. In addition, we broaden the class of multiphase situations we can deal with by coupling the FSL with an IT method. This extended methodology is demonstrated with cases of individual bubbles and droplets merging with a free surface.

1. Introduction

Dispersed flows are encountered in a broad spectrum of fields, and understanding their dynamics and how they affect the continuous phase is crucial for safe and efficient operation of many technical devices. For example, dispersed bubbly flow is the operational mode of bubble column reactors, which are widely used in chemical, biological, and petrochemical industries (Degaleesani et al., 2001), as well as in biological wastewater treatment (Prakash et al., 2001). Lagrangian particle tracking approach was successfully applied to simulate bubble column reactors in two and three dimensions, operating in laminar and turbulent flow regimes (Delnoij et al., 1997; Darmana et al., 2005; Buwa et al., 2006). In these models, a volume-averaged mass and momentum equations are solved for the continuum phase. Bubbles are tracked in Lagrangian fashion by solving Newton's second law of motion for each particle, or cluster of particles. Two-way coupling (i.e. bubbles' influence on the liquid) is accomplished via the liquid volume fraction and the interface momentum transfer incorporated as a source term in the momentum equations. One drawback of these

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https://doi.org/10.1016/j.ces.2017.10.037
0009-2509/

models is the limitation in the number of particles that can be tracked due to the available computer memory. Another drawback is the requirement that bubbles should be smaller than the grid cell size. This is because the liquid volume fraction for each cell should be strictly positive in order to solve the liquid-momentum equations. Furthermore, the mapping techniques used to transfer quantities, such as velocity and pressure gradient, between the Eulerian and Lagrangian frames require that the bubbles should be smaller than the grid cell size. For these reasons, simulations of bubble column reactors have used coarse meshes, so that the bubbles are smaller than the grid cell sizes. This poses problems for mesh refinement studies, bubbles' coalescence, and for simulating bubbles close to the walls where a fine mesh is required. A new methodology, which authors refer to as finite size Lagrangian (FSL) particle tracking, and inherits features of LPT and IT methods, was proposed to simulate finite-size bubbles whose diameter is larger than the grid cell but not well resolved for accurate IT (Badreddine et al., 2015). It was tested for a single air bubble rising in stagnant water and in linear shear flow with grid cell size ranges from five to twenty cells per bubble diameter. The results, in terms of bubbles' velocity, internal circulation, and the two-way coupling were in good agreements with results simulated with finely resolved interface tracking approach. In this work, the FSL method is extended to simulate finite-size bubbles or droplets impacting with a free surface. The simulation of a finite-size water droplet with a water surface is taken as a test case. The droplet was selected in purpose instead of a bubble to show the capability of FSL to simulate finite-size droplets. The finite-size droplet is simulated with FSL approach, and the free surface with an IT method. Once the droplet merges with the free surface, the whole system is solved with the IT. Then, simulations of a square bubble column reactor simulated using FSL are presented. Two different lift coefficients are tested, and results are compared to experimental data.

The outline of this paper is as follows: In Section 2, the FSL approach is summarized and the droplet coupling algorithm with the free surface is explained. Results of a droplet merging with the free surface simulated with FSL and compared to finely resolved IT are shown in Section 3. Simulation of bubble column reactor with FSL is also presented in Section 3. Finally, the conclusions are given in Section 4.

2. Numerical method

In this section, FSL approach is summarized. For a more comprehensive description, reader is referred to Badreddine et al. (2015). A single-set of governing equations based on Navier-Stokes equations is solved for the whole domain (including the bubbles), i.e. the single-fluid approach is used. It is formulated in terms of continuity and momentum equations, defined as:

$$\nabla \cdot \mathbf{u} = \mathbf{0}, \tag{1}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla \mathbf{p} + \nabla \cdot \mu(\nabla \mathbf{u} + \nabla^{\mathbf{T}} \mathbf{u}) + \rho \mathbf{g} + \mathbf{f_{cor}}, \tag{2}$$

where $\mathbf{f_{cor}}$ is the added correcting force. The mixture density ρ and viscosity μ are defined as:

$$\rho = \rho_l \phi + \rho_g (1 - \phi), \tag{3}$$

$$\mu = \mu_l \phi + \mu_g (1 - \phi), \tag{4}$$

where ϕ is the color function defined as liquid volume fraction, and the subscripts l and g correspond to liquid and gas phases, respectively. This means it is one in a cell fully in the liquid, zero in a cell fully in the gas. A smoothed sine profile for the interface is used:

$$\phi \equiv \phi_b = \frac{1}{2}\left(1 + \frac{d}{\tilde{\epsilon}} + \frac{1}{\pi}\sin\left(\frac{\pi d}{\tilde{\epsilon}}\right)\right), \tag{5}$$

where $\tilde{\epsilon}$ is taken to 1.5Δ, with Δ is the grid cell size, and d is the distance from the bubble's interface to the cell's center (xc, yc, zc):

$$d = \sqrt{(X_d - xc)^2 + (Y_d - yc)^2 + (Z_d - zc)^2} - R_b. \tag{6}$$

It should be noted that Eq. (5) is applied for interfacial cells with $|d| \leqslant \tilde{\epsilon}$, and it is valid for bubbly flows. In case of droplets, the liquid volume fraction $\phi \equiv \phi_{drop} = 1.0 - \phi_b$.

Since a staggered grid is used in this work, where the pressure and color function are defined at the center of the scalar cell, and the velocity components at the cell faces, the color function for the momentum cells is defined as an arithmetic average of the surrounding scalar cells. Bubbles' (or droplets) shape is imposed rather than calculated from the balance of surface tension with other forces acting on a bubble. A spherical shape is used. Therefore, the surface tension force is not included in the momentum equations. Thanks to this simplification, currents and small time increments required in models with surface tension force are avoided. The second feature of FSL is the introduction of the correcting force $\mathbf{f}_{cor}$ that is included in the momentum equations to reduce the error in the relative bubble velocity due to poor resolution of individual bubbles. It should be noted that this force is unnecessary for IT because the forces acting on the interface are resolved on the computational grid. The correcting force takes the following form:

$$\mathbf{f}_{cor} = \langle \rho \rangle \frac{\mathbf{V} - \langle \mathbf{u} \rangle}{\Delta t} \Phi_{disp}, \tag{7}$$

where $\langle \rho \rangle$ and $\langle \mathbf{u} \rangle$ are the volume-averaged density and velocity over the bubble (droplet) volume, respectively. This force is added to the cells that are inside the dispersed phase (bubbles or droplets), and it is taken into account by the dispersed volume fraction Φ_{disp}. For bubbles, $\Phi_{disp} = 1 - \phi_b$, and in case of droplets $\Phi_{disp} = 1 - \phi_{drop}$. Bubble's velocity is calculated from the hydrodynamic forces acting on it. These forces are theoretical with empirical correlations. The equation that governs the motion of the bubbles is Newton's second law given by:

$$\begin{aligned}(\rho_b + C_{AM}\rho_l)V_b \frac{d\mathbf{V}}{dt} = {} & (\rho_b - \rho_l)V_b \mathbf{g} + \frac{1}{2}\rho_l C_D \pi R_b^2 |\mathbf{u}_r| \mathbf{u}_r \\ & + C_L \rho_l V_b \mathbf{u}_r \times rot\, \mathbf{u}_l C_{AM} \rho_l V_b \frac{D\mathbf{u}_l}{Dt} \\ & - C_W \rho_l V_b (\mathbf{u}_r - (\mathbf{u}_r \cdot \mathbf{n}_w)\mathbf{n}_w)^2 \mathbf{n}_w,\end{aligned} \tag{8}$$

where the first term on the right hand side of the equation is the buoyancy force, the second the drag, the third the lateral lift force, the fourth added mass force, and the fifth term is the wall lubrication force. V_b is the volume of the bubble, and $\mathbf{n}_w$ is the wall normal vector. The added mass coefficient C_{AM} is taken to 0.5 and the wall force coefficient C_W proposed by Hosokawa and Tomiyama (2003) is used. The drag and lift coefficients will be specified for each simulation shown in the next sections. From these forces, the modeled bubble's velocity and bubble's center position can be computed using the first order explicit scheme. From the updated bubble's center position, the color function is recalculated using the assumption of spherical shape. In order to calculate the hydrodynamic forces, the undisturbed liquid velocity at the bubble's center is required. For LPT models, since the bubble is smaller than the grid cell size, the undisturbed liquid velocity is interpolated to the bubble's location from the grid resolved liquid velocity. An extension of this method was developed in FSL (Badreddine et al., 2015), and based on creating a pseudo cubic box of dimension $3R_b$ around each bubble (Fig. 1). The velocity components at the bubble's center are calculated by linear averaging the velocities at the faces' center of the pseudo-box. These velocities are determined (red and blue