Simulation of Droplet Dispersion in a Stirred Tank Using a Probability-Based Droplet Breakup Approach

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Highlights

- New approach for breakup in E-L simulation of droplet dispersion
- The simulation of breakup frequency insensitive to Lagrangian time step
- Sauter mean diameter and droplet size distribution are reasonably predicted
- Tortuosity is used for analyzing droplet trajectories

1. Introduction

Liquid-liquid dispersion in various stirred tanks is widely employed across industries such as pharmaceuticals, sewage treatment, and petrochemicals. While most related simulations are based on the Eulerian−Eulerian (E-E) approach for solving two-phase flow and population balance equations for droplet number density, the Eulerian−Lagrangian (E-L) approach allows for individual droplet motion tracking. However, its application is constrained by two primary challenges: computational load and droplet breakup modeling.

We have developed a GPU-accelerated Lattice Boltzmann method (LBM) and Large Eddy Simulation (LES) algorithm for transient simulation of single-phase flow in stirred tanks, achieving computational speeds on a GPU card 1500 times faster than those on 16 CPU cores [1-2]. In this study, we have further advanced this by developing a GPU-accelerated LBM-DPM model for the simulation of two-phase flow involving approximately 10^7 droplets.

Furthermore, we have introduced a novel droplet breakup approach based on probability to ensure the independence of breakup frequency on Lagrangian time step ($\mathrm{d}t_{\mathrm{drop}}$) in E-L simulations. The current droplet breakup approach in E-L simulations still relies on the breakup constraint ($d>d_{\mathrm{m}}$). After each Lagrangian time step, it is checked once to determine if the breakup constraint is satisfied. If so, the droplet will be permitted to break and generate smaller droplets. In present work, we proposed a novel droplet breakup approach based on probability. This approach eliminates concerns regarding the occurrence of non-integer or excessively small numbers of breakages associated with very small $\mathrm{d}t_{\mathrm{drop}}$.

2. Methods

In order to address the turbulence flow and the interaction of liquid and impeller in the stirred tank, we integrated the Lattice Boltzmann Method (LBM), coherent Large Eddy Simulation (LES), Immersed Boundary Method (IBM), and DPM. Within the Eulerian model, the continuous phase variables were solved using a GPU-accelerated LBM-LES algorithm, chosen for its computational speed and ability to resolve turbulent vortices. The interactions between the continuous phase and wall/impeller were modeled using IBM, leveraging its capacity to simulate complex boundaries. Meanwhile, in the Lagrangian model, droplet motion was represented by Newton's second law in DPM. We introduced a novel approach for implementing the breakup kernels as expressed as

$$g(\varepsilon, v) * \mathrm{d}t_{\mathrm{drop}} > x_{\mathrm{rand}} \tag{1}$$

where x_{rand} is a random number within the range of 0 to 1. $g(\varepsilon, v)$ with the unit s^{-1} represents the breakup kernel and is equivalent to the breakup frequency (f_{b}) for a droplet of volume v at a turbulence kinetic energy dissipation rate ε, i.e., $g(\varepsilon, v)=f_b$. The left side of Eq. (1) is less than 1 with a smaller $\mathrm{d}t_{\mathrm{drop}}$, and thus represents the breakup probability. When it exceeds x_{rand}, a breakup event occurs and is activated in our simulation.This approach ensures that the impact of $g(\varepsilon, v)$ remains consistent, irrespective of the value of $\mathrm{d}t_{\mathrm{drop}}$ utilized.

3. Results and discussion

The treatment of droplet breakup as an instantaneous process involves its implementation in each Lagrangian time step dt_{drop}, where a smaller dt_{drop} leads to a higher frequency of applying the breakup criterion, potentially altering the droplet breakup frequency. However, the sensitivity of droplet breakup frequency to dt_{drop} has not been addressed in the literature. In order to investigate the impact of dt_{drop} on droplet breakup frequency, the Eulerian time dt_{fluid} for the continuous phase and droplet size remain unchanged. Fig. 1 show that the spatio-temporal average breakup frequency $\overline{f_{bt}}$, simulated by the breakup criterion ($d>d_m$), exhibits a significant increase with dt_{drop}. Conversely, the new approach demonstrates insensitivity of the breakup frequency to dt_{drop}.

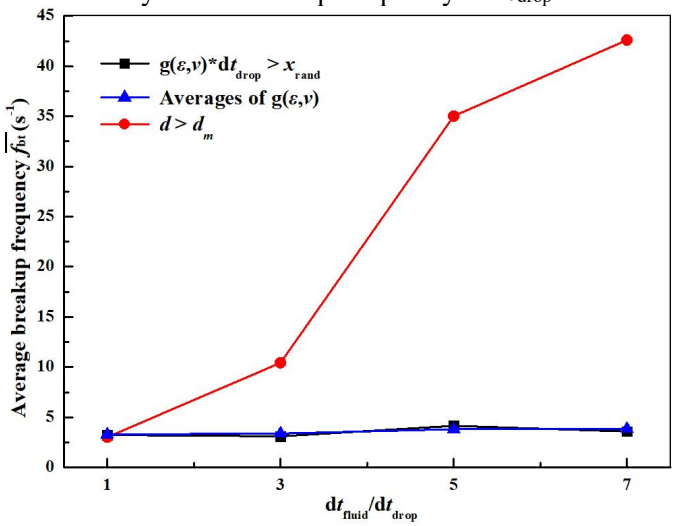

Figure 1. Effect of Lagrangian time step dt_{drop} on average breakup frequency.

4. Conclusions

The Eulerian − Lagrangian (E-L) simulation of droplet dispersion is constrained by computational load and the modeling of droplet breakup. To address the computational load, both the Eulerian and Lagrangian models were GPU-accelerated in this study. Besides, a novel approach for droplet breakup was introduced to ensure the independence of breakup frequency on the Lagrangian time step dt_{drop} and to mitigate long-term fluctuations in the spatio-temporal average breakup frequency. Furthermore, this new approach reasonably predicted the Sauter mean diameter and droplet size distribution.

References

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Keywords

Eulerian-Lagrangian method; droplet breakage; droplet trajectory; Lattice Boltzmann method