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Simulation of the multiphase flow in bubble columns with stability-constrained multi-fluid CFD models

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HIGHLIGHTS

- SCMF CFD models feature the use of stability condition to close two-fluid models.
- The lumped ratio of drag coefficient to bubble diameter is supplied by the new model.
- SCMF models offer better prediction without using empirical correlations or adjusting parameters.
- Phase separation into three fluids at the level of conservation equations is not necessary.
- Stability condition reflecting the compromise of two dominant mechanisms is the essence.

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ABSTRACT

The simulation of multiphase flow using multi-fluid CFD models is pertinent to the closure models for drag coefficient and bubble diameter, and empirical correlations or adjustable model parameters were inevitably needed. We proposed the stability-constrained multi-fluid models (SCMF) in our previous works based on the Dual-Bubble-Size (DBS) model and Energy-Minimization Multi-Scale (EMMS) concept. It utilized a stability condition to close the two-fluid models through the ratio of drag coefficient to bubble diameter. The stability condition reflects the compromise of two dominant mechanisms relevant to small bubbles or large bubbles. In this study, we further compared the three SCMF models with experiments and other multi-fluid models, i.e., the two-fluid models with Schiller-Naumann drag or Simonnet drag, the three-fluid model with Krishna drag, and the two-fluid model integrated with the population balance model (PBM). The SCMF models can offer better prediction without the need of empirical correlations or adjusting parameters for both the homogeneous and heterogeneous regimes. We further compared SCMF-A (gas and liquid phases), SCMF-B (dense and dilute phases) and SCMF-C (small bubble, large bubble and liquid) models. The three models are different in terms of the phase separation at the level of conservation equations. We found that SCMF-C cannot give further remarkable improvement, suggesting that the phase separation into three fluids at the level of conservation equations is not necessary, and the essential lies in the stability condition in the DBS model which reflects the compromise of two different dominant mechanisms represented by the two bubble classes. This may enhance our understanding on the mechanisms of scale separation in model developments.

1. Introduction

With the development of multiphase fluid dynamics, numerical algorithm and computational technology, computational fluid dynamics (CFD) is playing increasingly important roles in design and scale-up of multi-phase reactors. Among various multiphase CFD methods, the Eulerian-based two-fluid models, as a compromise between computational cost and accuracy, have been widely applied in multiphase flow simulations. The two-fluid model is essentially a kind of coarse-grained approach, averaging the single phase formulations and smoothing out the interfacial discontinuities between different phases. Hence the two-fluid model itself supplies only a framework of conservation properties of mass and momentum for two interpenetrating "continuous" fluids, whereas the micro- or meso-scale physics is hidden in the

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Nomenclature

b	breakup rate, s^{-1}
c	coalescence rate, $m^3 \cdot s^{-1}$
C_D	effective drag coefficient for a bubble around a swarm, dimensionless
c_f	coefficient of bubble surface area increase, dimensionless
d_b	bubble diameter, m
D_T	bubble column diameter, m
F^D	drag force, $N \cdot m^{-3}$
f_v	volumetric ratio of daughter bubble to its mother bubble, dimensionless
g	gravitational acceleration, $m \cdot s^{-2}$
$\boldsymbol{M}$	momentum exchange between phases, $N \cdot m^{-3}$
n	number density of the bubbles, m^{-6}
P_c	coalescence efficiency, dimensionless
S	source term in population balance equation, $m^{-6} \cdot s^{-1}$
$\boldsymbol{u}$	velocity vector, $m \cdot s^{-1}$
U_g	superficial gas velocity, $m \cdot s^{-1}$
$U_{g,L}$, $U_{g,S}$	superficial gas velocity of large bubbles or small bubbles, $m \cdot s^{-1}$
$\bar{u}_i$	bubble turbulent velocity, $m \cdot s^{-1}$
U_l	superficial liquid velocity, $m \cdot s^{-1}$
U_{tran}	superficial gas velocity at regime transition defined in the model of Krishna et al. $m \cdot s^{-1}$
V	bubble volume, m^3
V_b	bubble rise velocity, $m \cdot s^{-1}$
We_{ij}	Webber number, dimensionless

Greek letters

β	daughter bubble size distribution, dimensionless
ρ	density, $kg \cdot m^{-3}$
Γ	mass transfer between phases, $kg \cdot m^{-3} \cdot s^{-1}$
ε	energy dissipation rate, $m^2 \cdot s^{-3}$
ε_i	volume fraction, dimensionless
σ	surface tension, $N \cdot s^{-1}$
ω	bubble collision frequency, $m^3 \cdot s^{-1}$

Abbreviations

AF	acceleration factor
DBS	dual-bubble-size
SCMF	stability constrained multi-fluid
SF	scale correction factor
TFM-PBM	two-fluid model combined with population balance model

constitutive models by a cascading modeling approach [1]. The constitutive models usually involve the closure terms such as the interfacial forces (drag, lift, virtual mass, etc.) and the two-phase turbulence. Most of the closure models involve empirical correlations or parameters for engineering application, and the underlying micro- and meso-scale physics is difficult, if not impossible, to incorporate in the constitutive models.

For example, the average drag coefficient in CFD simulation is usually calculated from empirical correlations, or the single particle drag law corrected by a function of volume fraction of dispersed phase to consider the effects of bubble swarms. The correctors are also determined empirically and applicable for limited conditions. For instance, the Schiller-Naumann model [2] for particle-fluid systems was extended to the simulation of gas-liquid flows in some studies. Simonnet et al. [3] proposed a drag coefficient correlation based on the experimental measurements of quasi-two-dimensional bubble columns. Olmos et al. [4] reported that the corrector for drag coefficients should be used to achieve reasonable predictions, and the appropriate corrector varied with superficial gas velocity and bubble size. Yang et al. [5] reported that the correction factor not only varies with operating conditions and bubble diameter, but also with the standard drag coefficient models (C_{D0}) for single particle.

In our previous work [6,7], we have proposed a dual-bubble-size (DBS) model based on the Energy-Minimization Multi-Scale (EMMS) approach, including three simplified mass and force balance equations for two bubble classes and a stability condition. The stability condition was introduced to reflect the compromise between two dominant mechanisms: a liquid-dominant regime in which smaller bubbles prevail and tends to recirculate with liquid, and a gas-dominant regime favoring the existence of larger bubbles and gas disengagement. The stability condition is mathematically formulated as the minimization of the sum of two energy consumptions, and could provide a new physical constraint to conservation equations. With given operating conditions, this model can give the so-called structure parameters of a bubble column, qualitatively reflecting the trend of structure evolution and regime transition at macro-scale [6–8]. However, this model was only proposed as a zero-dimensional conceptual approach to explore the compromise of different mechanisms in the complex multiphase systems, applying only the simplified mass and force balance equations for the ensemble of the systems. It could not be directly used to calculate the spatial-temporal phase distribution and hydrodynamics.

We then proposed a stability-constrained multi-fluid (SCMF) approach for CFD simulation, applying the conceptual DBS model to derive some closure equations for drag coefficients in two-fluid models. In this way, the physics embodied in the stability condition could be incorporated into the current CFD framework. A drag model has been extracted from the DBS model and then integrated into CFD [5,9]. The results showed that the new drag model can improve the CFD simulation without any adjusting parameters.

A further analysis of the SCMF model was carried out by Xiao et al. [10]. The original two-fluid model equations for gas and liquid, together with the drag model derived from the DBS model, was enveloped and termed SCMF-A. For comparison, SCMF-B was proposed based on the two-fluid model equations for a dense phase (composed of liquid and small bubbles) and a dilute phase (large bubbles) and on the DBS drag model for large bubbles. In this model, the physics on the compromise of the two dominant mechanisms relevant to large bubbles and small bubbles was expected to be reflected not only at the level of closure drag models obtained from the DBS model, but also at the level of conservation equations. A step-by-step strategy was designed to ascertain the evolution from SCMF-A to SCMF-B. It suggested that the definition of the new two "fluids" in SCMF-B in terms of the differences in movement tendencies of the dense phase and the dilute phase, rather than the physical properties such as density and viscosity, was reasonable.

However, in the study of Xiao et al. [10], small bubbles were assumed to be homogeneously distributed in the so-called dense mixture phase, and the volume fraction of small bubbles in the dense phase was assumed to be constant for each computational