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Mesoscale Modeling of Multiphase Reactors: Concept, Theory and Applications

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Highlights

- Understanding the two mesoscales and their coupling is important.
- Stability condition reflecting compromise of dominant mechanisms provides a new constraint.
- The EMMS model has been integrated into CFD simulation for different multiphase systems.
- The stability-constrained CFD model shows much advantage over traditional closure models

1. Introduction

The increasing tempo of change in human life, society, economics and environment creates a correspondingly urgent need for scientists and engineers seeking for new perspectives for traditional problems some of which may be longstanding, or posing new questions and offering new answers. For example, although new catalysts and chemical technologies can be invented or patented in laboratory every year, process scaleup from laboratory to industrial application remains a troublesome or challenging issue. Successful cases are limited and risky, relying on the empirical correlations and the engineers whose knowledge and experience is acquainted through the long-term case study of previous well-established processes. It is generally acknowledged that the main technical problem, among others, is how to create an ideal transport environment for reactions and separation, and hence chemical reactions could be compatible with their carrier, i.e., the fluid flow, mass and heat transfer in multiphase reactors. A new angle to achieve a fundamental understanding and then seek efficient solutions of these classical problems is to reveal the mystery on mesoscales, i.e., the mesoscale transport phenomena and mechanisms relevant to bubbles, droplets and particles. Actually, mesoscale problems are essential to a more fundamental understanding of momentum, mass and heat transfer in the classical study of transport phenomena, and to the mixing, residence time distribution and rate-limiting analysis in the chemical reaction engineering, yet they are beyond the scope of those classical textbooks of chemical reaction engineering. Basically, there are two kinds of meso-scale problems in chemical reaction engineering, i.e., the mesoscales at the interfacial/material level and the mesoscales at the reactor level, each of which displays diverse mesoscale structures and phenomena, but some common principles may reside. Understanding the two mesoscale problems and their coupling is of great significance to the rational control and optimization of chemical processes[1-4].

2. Methods

Despite the complexity of mesoscale structures and mechanisms, we highlight a heuristic mesoscale modeling approach for multiphase reactor systems, starting from a conceptual Energy-Minimization Multiscale (EMMS) model and ending at the stability-constrained multifluid CFD model. While the stability condition determines the direction of system evolution, the stability-constrained CFD further describes the dynamics of structure evolution. By resolving the structures and dominant mechanisms, it is possible to establish a stability condition reflecting the compromise between different dominant mechanisms for multiphase reaction systems, and the stability condition supplies a mesoscale constraint in addition to mass and momentum conservation equations.

We establish the Dual-Bubble-Size (DBS) model, an extended EMMS approach for the gas-liquid flow in bubble column systems. The total energy dissipation in gas-liquid systems can be resolved into three parts, i.e., N_{surf}, N_{turb} and N_{break}. The former two are directly dissipated at microscales. The third reflects a kind of mesoscale energy dissipation, i.e, the energy stimulated from the interaction of turbulence eddies with bubbles and then stored temporarily as surface energy generated from bubble breakage and finally released to the liquid bulk phase during bubble coalescence. The mesoscale dissipation is used to sustain the formation and evolution of mesoscale structures and serves as a buffer for energy dissipation. Stability condition is formulated as the minimization of energy directly dissipated at microscales ($N_{\mathrm{surf}}+N_{\mathrm{turb}}\rightarrow\min$) or equivalently the maximization of energy consumption at mesoscales ($N_{\mathrm{break}}\rightarrow\max$). It reflects the compromise between two dominant mechanisms: $N_{\mathrm{surf}}\rightarrow\min$ represents a liquid-dominant regime and in this case larger bubbles are likely to break into those smaller bubbles which prevail in the system. $N_{\mathrm{turb}}\rightarrow\min$ represents a gas-dominant regime to favor the coalescence of smaller bubbles and the existence of larger bubbles. Stability condition in the DBS model is used to close the simplified conservation equations and hence the structure parameters can be obtained.

3. Results and discussion

Stability condition provides a mesoscale perspective to understand the flow regime transition at macroscale in bubble columns. The transition can be interpreted as the jump change of the global minimum point of micro-scale energy dissipation in the 3D space of structure parameters. The calculation of EMMS model demonstrates also that it is the stability condition that drives the structure variation and system evolution at macroscales, which may be the intrinsic similarity of gas-solid and gas-liquid systems. Theoretically stability condition may offer closure laws for CFD simulation, leading to the stability-constrained multifluid CFD model. While the direct integration is difficult, we propose various simplified approaches to derive the closure models for drag, bubble-induced turbulence and the correction factors for the kernel functions of bubble coalescence or breakup for population balance equations. The stability-constrained multifluid CFD model shows much advantage over current closure models. This theory is applied to gas-solid fluidization [5-6] and gas-liquid bubble column reactors, with further extension to gas-liquid-solid three phase flows and stirred tanks[7-9]. Several industrial applications on meso-scale modeling in liquid-solid polyethylene reactors and liquid-liquid emulsification systems will also be highlighted.

4. Conclusions

Mesoscale transport phenomena and mechanisms indeed offer new angles to achieve a more fundamental understanding on the traditional problems in chemical engineering. Despite these explorations and knowledge on mesoscales, mesoscale transport phenomena and mechanisms would continue to be a challenge for multiphase reaction systems. For example, there are currently no general guidelines to identify the dominant mechanisms and formulate the stability condition for different specific systems. Although we establish mesoscale models for gas-liquid and gas-solid systems, the presence of particles in gas-liquid-solid systems and the internals used to intensify the mixing in multiphase reactors have great influence on mesoscale structures, which requires further investigation. The adsorption of surfactant on bubble or droplet surface constitutes another mesoscale problem at the interfacial level, and it is necessary to bridge this mesoscale problem and the mesocale at the reactor level before we could completely understand the complexity of multiphase reaction systems.

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Keywords
Mesoscale; Computational Fluid Dynamics; Multiphase Flow; Reaction Engineering