Numerical Simulation of Bubble Column Reactors using a Hybrid Multiphase-CFD Approach

Hybrid Interface Resolving Two-Fluid Model (HIRES-TFM) by Coupling of the Volume-of-Fluid (VoF) method and the Two-Fluid Model (TFM)

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Introduction

Multiphase chemical reactors are widely used in chemical reaction engineering for a variety of processes, e.g. in the chemical, petroleum, metallurgical and energy industries [1]. The multiphase flows in some of these reactors, e.g. Bubble Column Reactors (BCR), are inherently complex in their underlying physical phenomena: their flow structures are intrinsically transient and characterized by very different spatial and temporal scales (figure 1), which have a strong influence on reactor performance, such as conversion, selectivity, site time yield, etc. It is therefore of paramount importance to develop both understanding and predictive simulation tools in order to obtain better and economically viable technologies for process intensification and optimization of these types of multiphase reactors in technical valuable terms of design or operating parameters.

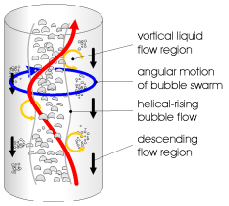


Figure 1: Schematic Flow Structures in Bubble Column Reactors according to [2]

State-of-the-art

In the past, knowledge of hydrodynamics and transport characteristics in bubble column reactors has been interpreted in the form of empirical correlations, which have numerous restrictions in terms of their validity for different operating conditions [1]. However, reliable BCR models that can be used with confidence for improving existing processes and scale-up of new processes are not yet available.

Recently, Computational Multi-Fluid Dynamics (CMFD) has emerged as a powerful tool for understanding the two-phase flows that occur in these types of reactors [3,4]. There is broad progress in the development and refinement of different numerical methods, each dealing with different flow types:

- interface resolving methods, e.g. the Volume-of-Fluid (VoF) method [5], are useful to study flow phenomena at the microscopic level by explicitly simulating the interface structure. However, due to the current limitations of computer capacity these approaches are limited to study the collective motion of only about 1000 dispersed fluid parts in a BCR.

The governing equation of the VoF-method are:
Continuity and momentum equation

$$\nabla \cdot \mathbf{U} = 0$$

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U}\mathbf{U}) = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \mathbf{U} + \nabla \mathbf{U}^T\right)\right] + \rho \mathbf{g} + \mathbf{F}_\sigma$$

where F_σ is the surface tension force, which can be modelled according to Brackbill et al. [6] or Lafaurie et al. [7].

Marker or indicator function (interface motion)

$$\frac{\partial \alpha_\varphi}{\partial t} + \nabla \cdot (\mathbf{U}\alpha_\varphi) = 0$$

where α_φ is the volume fraction of phase φ.
The fluid properties are

$$\mu = \alpha_a \mu_a + (1-\alpha_a)\mu_b \quad \text{resp.} \quad \rho = \alpha_a \rho_a + (1-\alpha_a)\rho_b$$

- averaging models, e.g. Two-Fluid Models (TFM) [8], are useful to study flow phenomena at the macroscopic level through the treatment of the coexisting phases as interpenetrating continua. Although these approaches are used for the simulation of the hydrodynamics of multiphase reactors, a large number of submodels is necessary to take into consideration both bubble-liquid interaction (including turbulence) and bubble-bubble interaction (including coalescence and break-up) in BCRs.

The governing equation of the TFM are:
Continuity and momentum equation

$$\frac{\partial \alpha_\varphi}{\partial t} + \nabla \cdot (\mathbf{U}_\varphi \alpha_\varphi) = 0$$

$$\frac{\partial \alpha_\varphi \mathbf{U}_\varphi}{\partial t} + \nabla \cdot (\alpha_\varphi \mathbf{U}_\varphi \mathbf{U}_\varphi) + \nabla \cdot (\alpha_\varphi \mathbf{R}_\varphi^{\text{eff}}) = -\frac{\alpha_\varphi}{\rho_\varphi}\nabla p + \alpha_\varphi \mathbf{g} + \frac{\alpha_\varphi}{\rho_\varphi}\mathbf{M}_\varphi$$

where M_φ is the interfacial momentum transfer term:

$$\mathbf{M}_\varphi = \underbrace{\mathbf{M}_\varphi^d}_{\text{drag force}} + \underbrace{\mathbf{M}_\varphi^l}_{\text{lift force}} + \underbrace{\mathbf{M}_\varphi^{vm}}_{\text{virtual mass force}} + \underbrace{\mathbf{M}_\varphi^w}_{\text{wall force}}$$

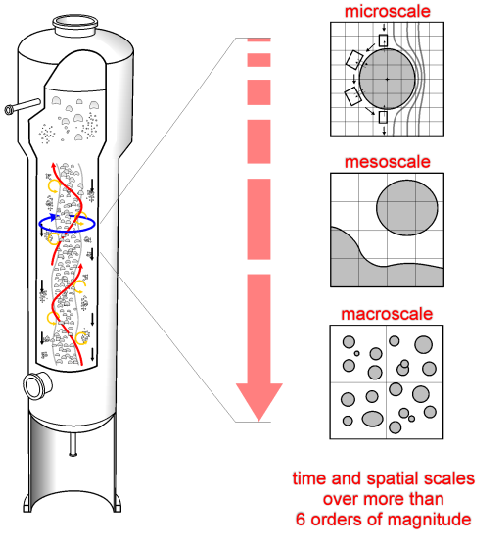
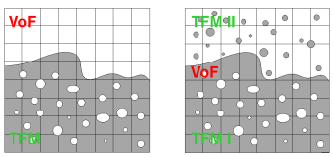


Figure 2: Physico-chemical Phenomena in Bubble Column Reactors

Challenge

The main challenge in CMFD is that phenomena occur over a wide range of scale, ranging from micro- over meso- to macroscale (multi-scale CMFD). Moreover, since typical industrial-scale bubble columns may contain many millions of bubbles, any developed multi-scale CMFD approach has to be emerged as large-scale CMFD tool – figure 2 – at acceptable computational costs and memory requirements.
In addition, for a proper description of reactive multiphase flows in bubble column reactors it would be necessary to combine the above mentioned methods for the simulation of different flow structures with models for mass transfer and reaction into one global multiphase reactor model.

An adaptive model concept would form a reasonable basis for the simulative description of both the fluid dynamics and reactor performance of bubble columns and would enable chemical and process engineers to comprehensive design and optimization studies of that kind of gas-liquid-reactors.



Two-Fluid-Model - dispersed flow region

- interfacial forces
- coalescence and breakup
- polydispersity
- turbulence incl. BIT
- mass transfer

Volume-of-Fluid Method - interface flow

- interfacial friction
- interfacial tension
- turbulence
- mass transfer
- resolution of interfacial structures and dynamics*

* local adaptive mesh refinement (AMR)

Figure 3: Concept and Features of HIRES-TFM

Conceptual Approach

For this purpose the two aforementioned two-phase flow models, which differ in treatment of multiphase phenomena, can be coupled: the interfaces of the dispersed phase(s) are modelled in the same way as in the classical TFM. Coincidently (in the same fluid domain) interfaces between continuous liquid and continuous gas phases are simulated with the VoF method as interface capturing technique. The basic features of this hybrid approach are given in figure 3.

Hybrid Interface Resolving Two-Fluid Model (HIRES-TFM)

The model, developed in this study, will be referred to as the Hybrid Interface Resolving Two-Fluid Model (HIRES-TFM), as it combines both methods in a coupled (hybrid) approach: the first part of the model is based on an interface resolving algorithm (VoF), which can be used only as long as the local computational grid density allows interface capturing. In a dispersed flow, where the dimensions of the particular fluid parts are comparable or smaller to the grid spacing, the interface capturing is not possible. Therefore, the second part of the model is the TFM based on averaged equations, which is more suitable for the simulations of a dispersed flow. Its accuracy does not depend so much on the grid density, but more on empirical correlations, which include the effects of the interface on the fluid motion.

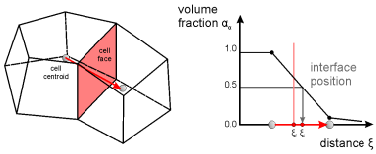


Figure 4: Calculation of Interface Position

The coupling of the two approaches is based on the volume fraction of the disperse phase (TFM) resp. the volume marker or indicator function (VoF):

$$\frac{\partial \alpha_a}{\partial t} + \nabla \cdot (\mathbf{U}_a \alpha_a) + \Gamma_d \nabla \cdot (\mathbf{U}_c \alpha_a (1-\alpha_a)) = 0$$

Note that the third term is an additional convection-based term which ensures compression of the interface but also is clearly conservative and maintains boundedness of α_a between 0 and 1 by $\alpha_a(1-\alpha_a)$ approaching 0 at both limits. In order to ensure the compression term does not bias the solution in any way it should only introduce flow of α_a normal to the interface, i.e. in the direction of $\nabla\alpha_a$.
The factor $\Gamma_d = f(\alpha_a, \nabla\alpha_a, \ldots)$ holds the switch criterion. It enables the switch between VoF ($\Gamma_d = 1$) and TFM ($\Gamma_d = 0$), as it carries information about the interface shape, quantifies the local dispersion of the two-phase flow structure and estimates the interface reconstruction correctness when applying the VoF method.
Appropriate models can be applied separately to both the dispersed flow regions and the interface region. In order to distinguish the regions, the calculation of the interface position is done by linear interpolation of the volume fraction α_a – see figure 4.

First results of gas-liquid flow in a cylindric column of 200 mm inner diameter are shown in figure 5. The iso-surface for α_a=0.5 represents the interface between the dispersed flow regions, while the contour plot shows the gas volume fraction in the bubbly flow.

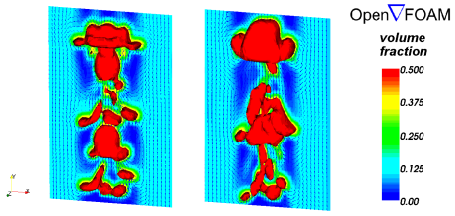


Figure 5: Simulation Result (prototype example)

Outlook

First results showed an extensive description of the fluid dynamics of operational states in gas-liquid reactors with bubbly flows and hence the possibility of a comprehensive design and optimization of that kind of gas-liquid reactors.

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