Advances in two and three-phase bubble columns modeling: large eddy simulation and population balance

Doctoral Dissertation Summary

Doctoral Program in Chemical Engineering (34.th cycle) – Politecnico di Torino

Advances in two and three-phase bubble columns modeling: large eddy simulation and population balance

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Bubble column reactors play a pivotal role in chemical engineering processes and plants, thanks to their well-known performance in mixing, heat and mass transfer and the simple operating mechanisms. However, despite this wide diffusion and well-established usage, the computational model of bubble columns is still challenging. The main reason is the complexity of the two- or, if solid particles are dispersed in the liquid medium, three-phase flows at industrial operating conditions, which are characterized by a deep reciprocal dependence of the phases behavior. In this perspective, several aspects, such as the accounting for phase inversion, the individual role of interfacial forces or the choice of the turbulence framework, are still nowadays among the most debated issues that require to be unambiguously addressed. Additionally, when the gaseous phase is injected at high velocity in the systems, the obtained bubbles dispersion is polydisperse with a wide distribution in the bubble size, affecting the main design parameters such as the gas hold up or the mass transfer coefficient. Moreover, the impact of solid particles in slurry bubble columns on these parameters is still ambiguous, and the corresponding computational model is even more difficult.

The latest research efforts have been focusing on tackling these issues but, however, every approach still strongly depends on the particular system which is considered, thus failing to extend the proposed solutions to a wider range of set-ups and conditions. This doctoral dissertation shares the efforts of the latest scientific production aiming to address the aforementioned issues but, on the other hand, aspires to individuate and develop one model with the widest applicability range. With this purpose, four different experimental set-ups were simulated, in order to strengthen the validity of the proposed model.

Firstly, it was urged the need for a fine modeling of phase interaction and phase inversion. This is fundamental to perform stable and fast simulations grounded on a physical phenomenon rather than on numerical artifices. To this purpose, the phase blending approach is described, including the tuning performed to identify the optimal parameters. It was then shown that, in the framework of a RANS description of the turbulence, which is, traditionally, the most popular for the modeling of bubble columns, this implementation leads to stabler and faster simulations without losses in results accuracy.

In parallel, the RANS turbulence description was also adopted to model a gas-liquid-solid bubble column with a square section. Slurry columns are particularly relevant in petrochemical processes since the solid particles in the liquid medium work as catalysts. The aim of this part of the work was the assessment of the role of the solid particles in hydrodynamics, phase interaction and bubbles coalescence and breakage. In this case, the inclusion of secondary interfacial forces was necessary to maintain the stability and accuracy of the simulations, probably due to the square geometry of the column. Under this basis, the model successfully predicted the behavior of the flow following the addition of solid particles, which resulted in a lower gas hold-up and a larger mean bubble size due to the promoted coalescence induced by the solid particles, in line with experimental observations.

Secondarily, the phase blending model was implemented together with a LES turbulence description. This was a novelty compared to the latest scientific research, that, in the context of the modeling of bubble columns, mainly applied LES to simplified geometries and operating conditions. In this work, different systems at high gas velocity were simulated and, in particular, the condition of asymmetrical gas injection was investigated in detail. An analysis of the various models for the calculation of the subgrid turbulent eddy viscosity was then performed, suggesting that the classical Smagorinsky model, coupled with the inclusion of the bubble induced turbulence effects, could be the most reliable model for describing bubbly flows at these conditions. Afterwards, the impact of the lift force was assessed. Results showed that its inclusion in the set of interfacial forces does not contribute to an improvement of the results, and, in the asymmetrical injection conditions, it even produces significant miscalculation in the prediction of the flow.

A population balance modeling is then implemented in the LES turbulence framework to estimate the bubble size distribution: to the best of our knowledge, coupled LES-PBM models have not been applied so far to the simulation of bubble columns. Results confirm once more the considerable potential of the LES approach for the modeling of bubble columns: the estimated bubble size distribution matches thoroughly the experimental measurements. Coupled LES-PBM simulations were performed to compute the oxygen mass transfer coefficient in a square bubble column where pure and contaminated water was used as liquid phases: in particular, the latter consists in water - Sodium Dodecyl Sulfate solutions with different concentrations of the contaminants. Once more, the model successfully predicted both the flow patterns and the mass transfer coefficient in all the tested conditions, confirming the experimental measurements and, specifically, it was reported an increase in the mass transfer coefficient with the addition of the contaminant to the liquid phase. Additionally, the adoption of the LES turbulence framework allowed to solve the issues originated from the square geometry and reported in the RANS simulations of the slurry column without any additional modeling assumptions.