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Simulation of polydispersed multiphase systems with Computational Fluid Dynamics and Population Balance Modeling using open source codes

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Highlights

- A CFD-PBM methodology is developed and extensively validated.
- QBMM are used to solve the GPBE.
- The methodology is implemented in the open source code OpenFOAM.
- Gas-liquid and liquid-liquid systems are investigated.

1. Introduction

The design and the optimization of turbulent multiphase equipment are very common tasks in the chemical, pharmaceutical, food and process industries. Turbulent flow conditions, under which most of these processes work, are essential to improve the overall performance, enhancing heat and mass transfer rates.

The approach historically adopted for the design and scale-up of multiphase systems is based on the use of empirical correlations, often formulated through costly and time-consuming experimental campaigns. However, this approach might have several limitations: 1) the range of validity of such correlations is limited to specific vessel geometries and operating conditions, 2) these correlations are usually based on the hypothesis that the system is well-mixed, neglecting the effect of spatial inhomogeneities often identified even on small scale systems.

These limitations can be overcome by means of the numerical simulation with the Computational Fluid Dynamics (CFD) and the Population Balance Modeling (PBM). In fact, by coupling these two modeling approaches, it is possible to obtain a fully-predictive methodology capable of describing different systems and geometries working under different operating conditions. Such coupling has been carried out within the open source CFD framework OpenFOAM, leading to a computational tool able to properly predict local and global properties of gas-liquid and liquid-liquid systems. Moreover, the development of open source modeling tools facilitate the cooperation between academic institutions and the involvement of Small and Medium Enterprises, due to favorable conditions in terms of software license. In this contribution, recent results in terms of model development and validation are presented, with particular attention to reactive systems where the detailed knowledge of the interfacial area and the driving force of the mass transfer can be achieved.

2. Methods

The numerical simulation of large scale multiphase systems can be performed by using the Eulerian-Eulerian approach, in which the continuous and the disperse phases are treated as interpenetrating continua, sharing the same portion of physical volume. Predictions of the physical reality can be achieved with this approach only if mass, momentum and energy phase coupling are successfully described, meaning that the model should acknowledge the fact that each dispersed particle may have different size, velocity, temperature and chemical composition. The evolution in space and time of such distribution is dictated by the so-called Generalized Population Balance Equation (GPBE) [1], in which the momentum, heat and mass exchange with the continuous phase, as well as particle coalescence and breakage, can be taken into account with specific mesoscale models. The selection of proper mesoscale models is therefore of crucial importance for the physical prediction of the relevant properties of system under investigation. A computationally efficient approach for solving the GPBE is represented by the Quadrature-Based Moment Methods (QBMM), where the evolution of the entire particle population is recovered by tracking a few low-order moments of the

distribution, allowing to simultaneously account for the fluid and population dynamics in a reasonable computational time. As previously mentioned, the implementation of the QBMM has been carried out in the open source CFD code OpenFOAM, with particular attention to preserve important properties of the moments, such as the conservation, boundedness and realizability [2].

3. Results and discussion

An example of the information that can be obtained from the presented methodology are shown in Figure 1, where the contour plots of different quantities are depicted [3,4,5]. As it is possible to observe, the simulation can give the modeler useful details to design new equipment or optimize, scale-up, scale-down existing processes, providing a qualitative and quantitative analysis not only on the fluid dynamics behavior of the systems, but also on the evolution of the disperse particles and the chemical reactions. This latter information is indeed very useful to predict the heat and mass transfer rates, with a potential impact on the process design and development.

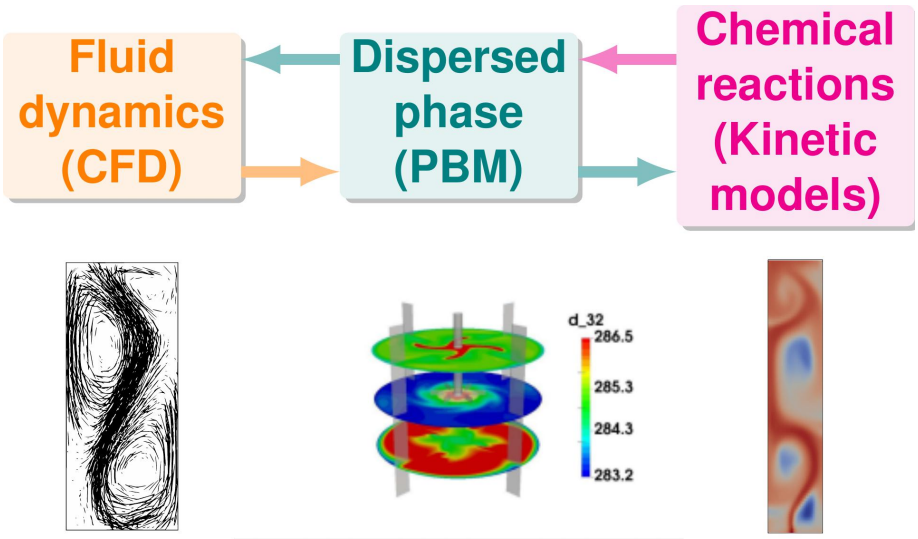

Figure 1. First row: block diagram showing the interdependency between different parts of the methodology. Second row: examples of plots for different interesting quantities. From left to right: flow field inside a bubble column [3], mean droplet Sauter diameter inside a liquid-liquid stirred tank [4] and concentration of a reaction product inside a reactive bubble column [5].

4. Conclusions

In this work, a fully-predictive methodology that couples the CFD and PBM for the simulation of reactive gas-liquid and liquid-liquid systems is developed. This methodology has been implemented into the open source CFD code OpenFOAM, which has the advantages of being easily customizable and distributed under GPL. The QBMM are suitable to solve the GPBE coupled with the fluid dynamics description of the multiphase flow and the kinetic models of the chemical reactions. An extensive validation of the model has been carried out by considering numerous test cases, i.e., different geometries working under different operating conditions. The predictions provided by this tool can reduce the costs related to the process design, development and optimization.

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Keywords
Computational Fluid Dynamics; Population Balance Modeling; open source codes; OpenFOAM.

CV for the Gianni Astarita Young Investigator Award

Antonio Buffo is currently assistant professor at the Department of Applied Science and Technology of Politecnico di Torino. His research work focuses mainly on the simulation of multiphase systems, in particular on the fluid dynamic characterization of dispersed systems (e.g., bubbly flows and emulsions). The computational tools developed combine computational fluid dynamics (CFD) and population balance modeling (PBM) for the description of macro and micro scale phenomena, and their influence on mass, momentum and heat transfer and chemical reaction rates. He authored more than 30 papers in international journals or conference proceedings. He took part in numerous industrial projects (ENI S.p.a, Rockwood, BASF SE, VTT) and he currently cooperate with other institutions (Massachusetts Institute of Technology, Warsaw Institute of Technology, Aalto University, Technical University of Eindhoven, Helmholtz-Zentrum Dresden-Rossendorf).

Research and Work Experience:

- *December 2016-present:* Assistant professor at the Department of Applied Science and Technology of Politecnico di Torino in the institute of Chemical Engineering.
- *January 2015-December 2016*: Post-doctoral researcher at Aalto University (Finland), working on modeling of reactive polydisperse liquid-liquid systems, through Computational Fluid Dynamics (CFD) and population balances (Consortium ExtraFin - PORLIS Project). Research funded by Academy of Finland.
- *January 2012-December 2014*: Post-doctoral researcher at Politecnico di Torino, working on the implementation and validation of population balance models in the open-source CFD code OpenFOAM for gas-liquid systems. Research funded by BASF (Ludwigshafen, Germany).

Education:

- *January 2010-January 2013:* Ph.D. in Chemical Engineering Dissertation title: "Multivariate population balance for turbulent gas-liquid flows Advisors: Prof. Daniele Marchisio, Prof. Marco Vanni
- *October 2007-December 2009:* M.D. cum laude in Chemical Engineering Thesis title: "Mass transfer modeling in gas-liquid stirred tanks through Computational Fluid Dynamics and Population Balances" (in Italian).

Awards:

- Highly cited paper cited papers published in International Journal of Multiphase Flow: Multivariate Quadrature-Based Moments Methods for turbulent polydisperse gas-liquid systems, 2013.

Selected publications:

1. A. Buffo, V. Alopaeus, A novel simplified multivariate PBE solution method for mass transfer problems, Chemical Engineering Science 172 (2017) 463–475
2. A. Buffo, M. Vanni, P. Renze, D.L. Marchisio, Empirical drag closure for polydisperse gas–liquid systems in bubbly flow regime: Bubble swarm and micro-scale turbulence, Chemical Engineering Research and Design 113 (2016) 284–303
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