The 3rd International Conference on Numerical Methods in Multiphase Flows, ICNMMF-III
June 26-29, 2017, Tokyo, Japan

Direct Numerical Simulation of Bubbly Flows

Holger Marschall[*‡1], Daniel Deising[1], Chiara Pesci[1], Xuan Cai[2],
Martin Wörner[2], Olaf Deutschmann[2], Dieter Bothe[1]

[1] Mathematical Modeling and Analysis, Technische Universität Darmstadt, Germany
[2] Institute for Catalysis Research and Technology, Karlsruhe Institute of Technology (KIT), Germany

*two-phase DNS, bubbly flows, transport processes,
sharp-interface model, diffuse-interface model.*

For Direct Numerical Simulation (DNS) of bubbly flows on unstructured meshes of general topology (i.e. polyhedral meshes) we discuss the method-inherent numerical advantages of three main representatives of DNS methods based on sharp-interface modeling, namely the volume-conservative Volume-Of-Fluid (VOF) interface capturing method, the area-conservative Arbitrary Lagrangian-Eulerian (ALE) interface tracking method and the Level-Set (LS) front tracking method. Likewise, the two main representatives within the diffuse interface modeling framework, namely the two-phase Allen-Cahn and Cahn-Hilliard phase-field methods, are considered regarding their specific potential for DNS of bubbly flows.

Figure 1 Single rising bubble under the influence of surfactant.

The main purpose of this talk is to discuss these distinct DNS methods regarding their capabilities to cope with different transport problems in bubbly flows, imposing various (additional) numerical challenges upon the underlying methods. All mentioned DNS methods have been implemented into a single C++ development platform for Computational Continuum Mechanics and Multiphysics: OpenFOAM – Open Field Operation And Manipulation [1, 2]. As a consequence, there is now conceptual freedom to employ the particular DNS method, which exhibits advantageous properties with respect to desired numerical requirements being specifically imposed by interfacial transport problems.

In particular, this contribution is devoted to the following transport processes occurring in bubbly flows and their DNS by means of suitable sharp- or diffuse-interface methods:

surfactant transport at bubble interfaces (cf. Fig. 1) – i.e. the transport of surfactant on the bubble interface and in the bulk, which is coupled via sorption processes resulting in a multi-equation/multi-region coupling problem. In particular, we will focus on numerical modeling of the two limiting sorption regimes, namely diffusion-controlled (fast) and kinetically-controlled (slow) adsorption, which necessitate substantially different numerical treatments. We have developed a comprehensive framework for numerical modeling of interfacial transport of soluble and insoluble surfactants [3, 4] within the framwork of the Arbitrary Lagrangian-Eulerian (ALE) Interface-Tracking method based on OpenFOAM interTrackFoam solver family.

interfacial mass transfer across bubble interfaces – In general, numerical methods for interfacial mass transfer mainly suffer from numerical difficulties due to the concentration jump across the interface, which needs to be accurately captured, and from large concentration gradients at the interface, which need to be resolved. Here, we employ an

‡ Corresponding Author: Holger Marschall (marschall@mma.tu-darmstadt.de)

algebraic Volume-Of-Fluid (VOF) method based on OpenFOAM's interFoam solver family. The species transfer is consistently incorporated through a novel single-field model named 'Continuous Species Transfer' (CST) model [5, 6]. The CST approach can be seen as an enhancement of the original model proposed by Marschall et al. [5], which consistently combines their findings with the one-field equation derived by Haroun [7] into a unified single field model for interfacial species transfer, cf. [6] for details.

bubble wetting in complex domains – This part of the talk focuses on wetting physics at internals of bubble columns, particularly considering complex novel geometries such as periodic open cell structures and porous media, where phase-field methods are advantageous since they do not suffer from the so-called moving contact line paradoxon of sharp interface approaches, which is a non-integrable stress singularity near a moving contact line due to no-slip conditions at the wall. We have developed a unified solver framework for two-phase phase-field methods [8, 9] within OpenFOAM, entitled phaseFieldFoam. Significant use of OpenFOAM's technology, e.g. its block-coupled matrix support for simultaneous solution of two 2nd order Helmholtz-type transport equations (from decomposition of the 4th order Cahn-Hilliard equation) and the Finite Area Method for discretisation of a dynamic contact angle model based on the wall energy relaxation approach, has been found mandatory for a consistent, accurate and robust Finite Volume based phase-field solution method.

Summarizing, this talk will be concerned with the theoretical foundation of the main representatives of two-phase DNS approaches for bubbly flows as well as with method-inherent numerical challenges of both sharp-interface capturing and tracking methods and diffuse-interface phase-field methods. We will further briefly highlight our developments within the OpenFOAM C++ library with focus on capabilities of the developed DNS methods to cope with interfacial transport processes and associated physico-chemical phenomena, while also clearly addressing the need for further developments and research in this field.

REFERENCES

[1] H. G. Weller, G. Tabor, H. Jasak, and C. Fureby. A tensorial approach to computational continuum mechanics using object orientated techniques. *Comput. Phys.*, 12(6):620–631, 1998.

[2] H. Jasak, A. Jemcov, and Ž. Tukovic. OpenFOAM: A library for complex physics simulations. In *International Workshop on Coupled Methods in Numerical Dynamics IUC*, Dubrovnik, Croatia, September, 19-21 2007.

[3] K. Dieter-Kissling, H. Marschall, and D. Bothe. Numerical method for coupled interfacial surfactant transport on dynamic surface meshes of general topology. *Computers & Fluids*, 109:168–184, 2015.

[4] C. Pesci, K. Dieter-Kissling, H. Marschall, and D. Bothe. *Computational Methods for Complex Liquid-Fluid Interfaces*, chapter Finite Volume/Finite Area Interface-Tracking Method for Two-Phase Flows with Fluid Interfaces Influenced by Surfactant, page 538. Progress in Colloid and Interface Science. CRC Press, Taylor & Francis Group, December 2015. ISBN 978-1-4987-2208-7.

[5] H. Marschall, K. Hinterberger, C. Schüler, F. Habla, and O. Hinrichsen. Numerical simulation of species transfer across fluid interfaces in free-surface flows using OpenFOAM. *Chem. Eng. Sci.*, 78(0):111–127, 2012.

[6] D. Deising, H. Marschall, and D. Bothe. A unified single-field model framework for Volume-Of-Fluid simulations of interfacial species transfer applied to bubbly flows. *Chem. Eng. Sci.*, 139:173–195, 2016.

[7] Y. Haroun, D. Legendre, and L. Raynal. Direct numerical simulation of reactive absorption in gas-liquid flow on structured packing using interface capturing method. *Chem. Eng. Sci.*, 65(1):351–356, 2010. 20th International Symposium in Chemical Reaction Engineering–Green Chemical Reaction Engineering for a Sustainable Future.

[8] X. Cai, H. Marschall, M. Wörner, and O. Deutschmann. Numerical simulation of wetting phenomena with a Phase-Field method using OpenFOAM. *Chem. Eng. Technol.*, 38(11):1985–1992, 2015.

[9] X. Cai, H. Marschall, M. Wörner, and O. Deutschmann. Numerical study on the wettability dependent interaction of a rising bubble with a periodic open cellular structure . *Catalysis Today*, 273:151–160, 2016.