Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Modeling and Numerical Simulation of Species Transfer in Bubbly Flows Using OpenFOAM

Researchers
Dr.-Ing. Holger Marschall and Daniel Deising

Principal Investigator
Prof. Dr. Dieter Bothe

Project Term
2017 - 2018

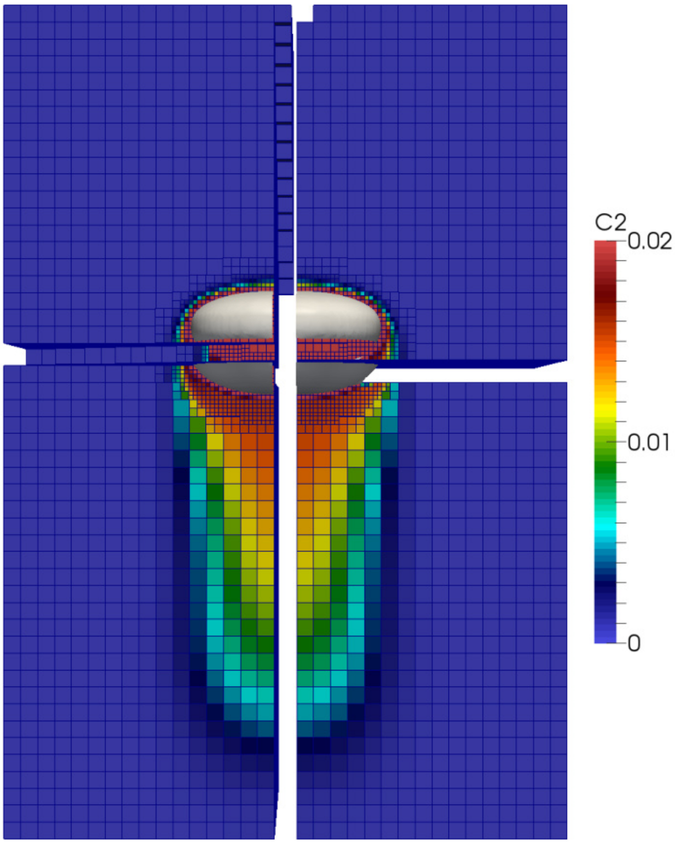
Project Areas
Materials Engineering, Mathematics

Clusters
Lichtenberg Cluster Darmstadt

Software
OpenFOAM

Institute
Mathematical Modeling and Analysis

University
Technische Universität Darmstadt



Introduction

The aim of our study is the deduction of an improved interfacial species transfer closure to be further used in bubble column simulations utilizing a two-fluid model. To arrive at such a closure, our research focuses on the Direct Numerical Simulation (DNS) of species transfer at rising single bubbles and bubble groups from the gas phase into the liquid phase. For our simulations, we employ a Volume-of-Fluid (VoF) method based on the OpenFOAM interFoam solver. The species transfer is simulated using a novel single field model named ‚enhanced Continuous Species Transfer (CST)‘ model[1] , which is based on the works of Marschall et al.[2] and Haroun[3].

Methods

In the simulation of rising single bubbles, we follow the bubble by employing a moving reference frame technique. The bubble swarms are mimicked by a bubble group in a fully periodic domain (pseudo swarm). The numerical implementation has been accomplished in the OpenFOAM C++ library for computational continuum mechanics, hence, it supports arbitrary unstructured meshes including dynamic adaptive mesh refinement (AMR) around the interface and a dynamic load balancing technique, which are employed to enhance the performance in parallel computations (HPC aspect! See figure). Algebraic advection of volumetric phase fraction and species concentration are based on Interface Capturing Schemes for consistency. The corresponding solvers were found to be accurate and robust with a comprehensive set of numerical benchmarks and validation test cases for realistic transport and material properties, i.e. realistic Schmidt numbers, diffusivity ratios and Henry coefficients. Further, a study of species transfer from single rising bubbles for different fluid properties was started, to obtain a closure relation for mass transfer which includes the influence of bubble shape. This influence is only briefly studied in literature,[4] although it has a significant influence onto the interfacial mass transfer.

Results

Our main focus in recent history was the model development, implementation and validation for simulating species transfer in context of algebraic VoF methods. The future focus will be on high performance computing, simulating interfacial species transfer at rising single bubbles and bubble groups by means of DNS to arrive at a closure model for mass transfer. We gratefully acknowledge the financial support from BMBF project ‚Multiscale Modeling of Multiphase Reactors (Multi-Phase)' (FKZ: 01RC1102).

Figures

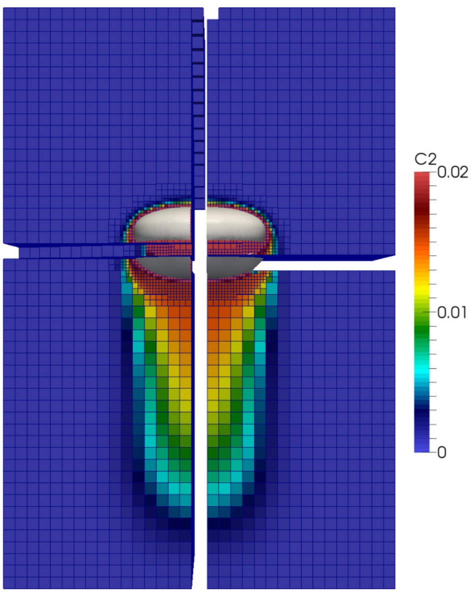


Figure 1: AMR and load balancing.

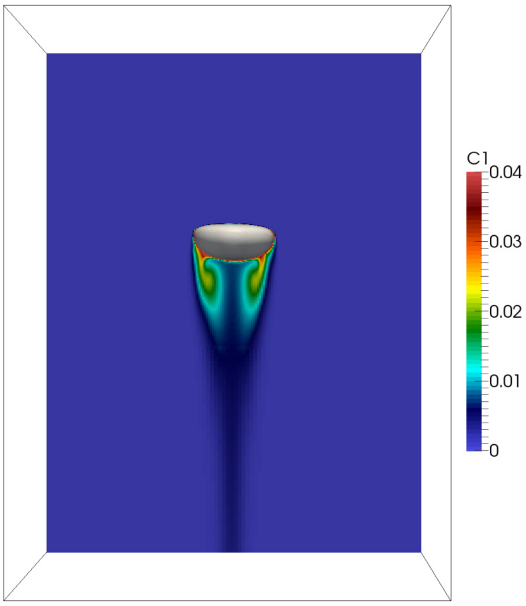


Figure 2: Species concentration (Pe=1000).

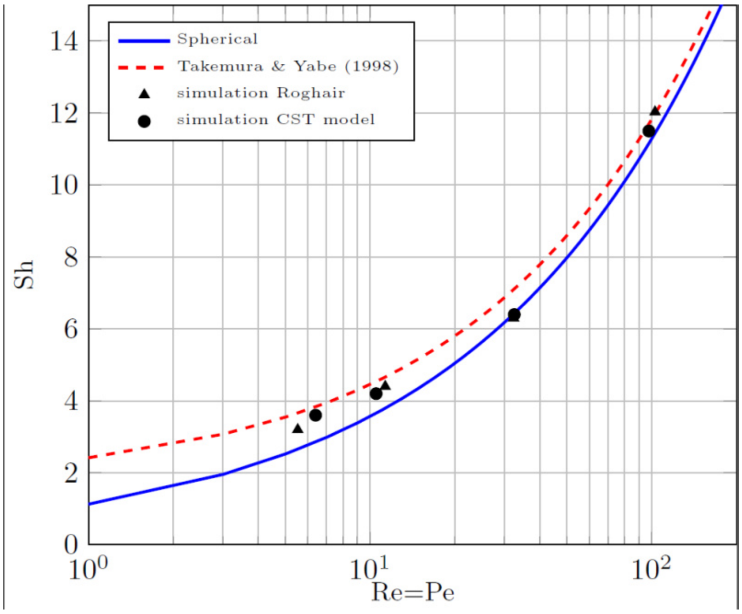


Figure 3: Sherwood correlation comparison.

Reference

1. D. Deising, H. Marschall, and D. Bothe (2014), A unified single-field model framework for Volume-of-Fluid simulations of interfacial species transfer applied to bubbly flows. Submitted to Computers and Chemical Engineering. http://dx.doi.org/10.1016/j.ces.2015.06.021

2. H. Marschall et al. (2012), Numerical simulation of species transfer across fluid interfaces in free- surface flows using OpenFOAM. Chemical Engineering Science78: 111-127. http://dx.doi.org/10.1016/j.ces.2012.02.034

3. Y. Haroun, D. Legendre, and L. Raynal (2010), Volume of fluid method for interfacial reactive mass transfer: Application to stable liquid film. Chemical Engineering Science65: 2896-2909. https://doi.org/10.1016/j.ces.2010.01.012

4. A. C. Lochiel, P. H. Calderbank. 1964. Mass transfer in the continuous phase around axisymmetric bodies of revolution. Chemical Engineering Science 19, 471- 484. https://doi.org/10.1016/0009-2509(64)85074-0

Last Update: 2022-07-14 23:29