Numerical Simulation of Species Transfer at Gas-Liquid Interfaces using OpenFOAM®

Concept of the Continuous-Species-Transfer (CST) Method

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Abstract

1. Introduction

Detailed understanding of physico-chemical phenomena at gas-liquid interfaces are of pivotal interest in chemical reactor engineering when addressing the optimization and process intensification of multiphase apparatus and reactors.

2. State-of-the-Art

Recently Computational Multi-Fluid Dynamics (CMFD) has emerged as a powerful tool for understanding free-surface flows in multiphase reactors [1]. However, the main problem in CMFD is that phenomena occur over a wide range of scale (multi-scale CMFD).

The numerical simulation of i.e. species transfer across fluid interfaces is a severe challenge to existing CMFD methods. They mainly suffer from numerical difficulties due to both the steep concentration gradient (at high Schmidt numbers), that needs to be resolved down to the Batchelor length scale, and a sharp concentration jump (at high Henry coefficients) occuring at the interface due to different species' solubilities.

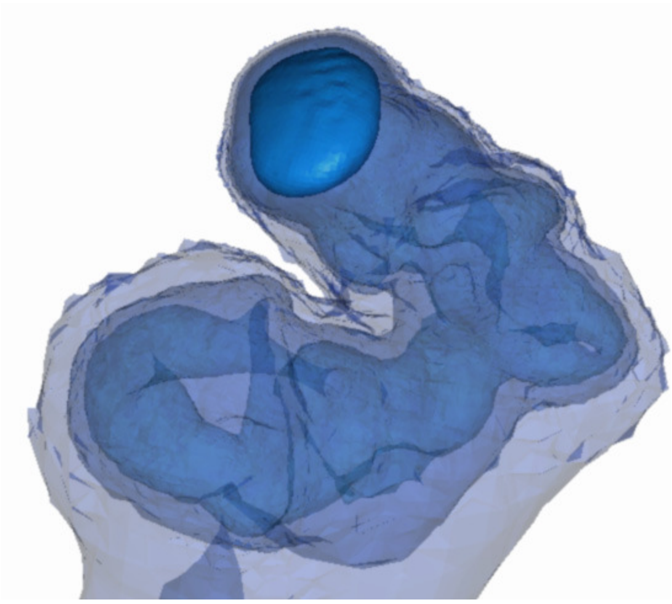

Figure 1 Rising air bubble and its oxygen concentration wake in surrounding water

3. Conceptual Approach

In order to overcome these problem, a continuum mechanic modeling approach of solubility and species transfer was used. This enables to convert Henry's law into a solubility flux over the fluid interface. Therefore, the concentration jump is converted into a continuous effect spread over several interfacial cells, as it is a well-established practise in Volume-of-Fluid Methods for the momentum jump due to the surface tension force at gas-liquid interfaces known as Continuous-Surface-Force (CSF) Method [2].

We corrected and developed the original continuous approach [3] further towards a Continuous-Species-Transfer (CST) Method that accurately describes both the topology (normal, curvature) of the fluid interface and the local species flux across it. In addition, we use a multivariate convection scheme in order to account for an arbitrary number of species crossing the fluids' interfaces at concentration levels ranging over several orders of magnitude. Furthermore, an adaptive mesh refinement (AMR) and moving frame of reference (MFR) technique was adopted in order to (efficiently) provide sufficient local mesh resolution to capture both species concentration gradients and the interfacial topology of the free-surfaces.

4. Results

A basic test case for validation of the new CST method will be presented. It consists of a cube with an unit edge length of 1 cm, one half each initially filled with air and water, respectively. There is no convective species transfer in the fluids present, since all boundaries of the fluid domain are modelled using the free-slip boundary condition, and both air and water are initialized as quiscient fluids throughout the domain. Furthermore, wetting effects are neglected using a static contact angle which is set to 90°. Further, species concentration is initialized equally distributed within the liquid phase using a normalized concentration of $\bar{c} = 1$. Comparison between the exact and the approximative solutions demonstrates very good agreement of numerical simulation results and expected concentration fields for this basic validation test cases.

Further the application of the CST method will be discussed. Exemplary Figure 1 shows an air bubble with its oxygen concentration wake due to species transfer from the bubble to the continuous phase while rising through quiescent liquid. Species transfer is considered for a air-water system, e.g. at high liquid Schmidt number of $Sc \approx 500$ and Henry coefficient of $He = 33$.

Key words: interfacial species transfer, interface capturing, Volume-Of-Fluid Method, Henry's law, two-phase flow

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