

Direct Numerical Simulation of Species Transfer in Bubbly Flows

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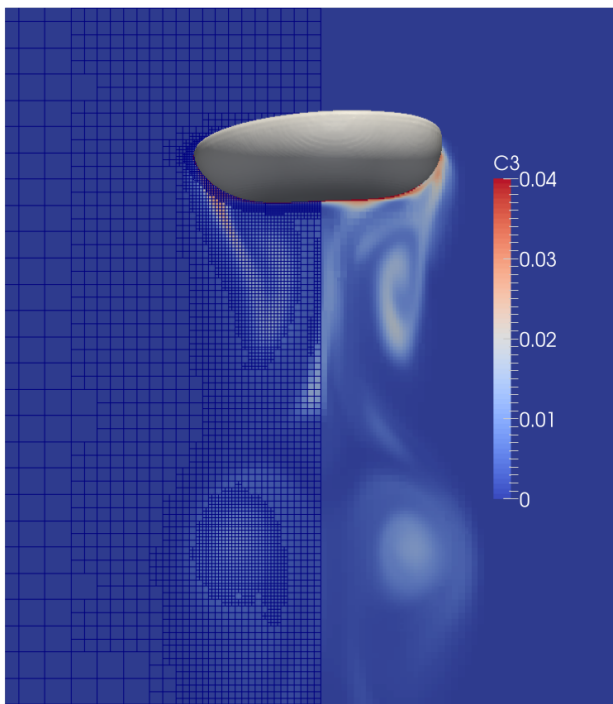
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This contribution is dedicated to species transfer modeling at fluid interfaces in context of algebraic Volume-of-Fluid (VoF) methods. The central challenges in capturing the species transfer over fluid interfaces by Direct Numerical Simulations (DNS) are the steep concentration gradients at the interface and the abrupt interfacial concentration jumps, which impose severe requirements onto the underlying numerical methods. Therefore, a novel method for simulating species transfer in two-phase flow systems in context of algebraic Volume-of-Fluid methods has been developed with regard to above method requirements, the so-called Continuous Species Transfer (CST) method [1,2,4]. In the developed approach, the mass transfer is included in form of a single-field formulation derived by the framework of conditional volume averaging. The interface jump and transmission conditions are herein transferred into an additional diffusive term in the interfacial region. Validity of the method is for dilute species without (or with negligible) phase change. The spatial discretization on unstructured meshes of general topology is considered by including bounded (semi-) implicit skewness correction methods [3]. The derived CST model ensures mass conservation and boundedness of the concentration fields and allows for a fully implicit discretization of the diffusive transport and interfacial transfer, thus increasing numerical stability and overcoming explicit time step limitations.

High Performance Computing

To resolve the thin concentration boundary layer, high performance computing techniques are utilized in this work, namely dynamic adaptive mesh refinement (AMR) and dynamic load balancing techniques to locally increase the resolution in regions of interest (here, gas-liquid interface; cf. Figure 1) and efficiently use the computational resources. These techniques, being generally available within the OpenFOAM framework, have been substantially enhanced in course of our research. This required e.g. the implementation of a new surface mapping algorithm and a clustered decomposition method which allows for consistent decomposition of the refinement history, a list containing information about the connection of parent (base mesh) and child cells (locally refined mesh). Further, a multi-criterion

refinement library based on [5] has been developed which allows the user to specify a multitude of different refinement criteria and assign to each a specific refinement target level. The multi-criterion refinement dictionary used to specify the computational mesh shown in Figure 1a is given in Figure 1b. Here, the different criteria contain triples where the last number specifies the refinement level for this criterion and the other two define the value range to mark cells for refinement.



(a) Concentration field around single rising bubble with computational mesh.

```
dynamicFvMesh    dynamicRefineBalancedFvMesh
refinementControls
{
    enableRefinementControl    true;
    interface
    (
        alpha1 (2 5)
    );
    fields
    (
        alpha1 (0.01 1.1 3)
        C1     (0.001 0.05 2)
    );
    gradients
    (
        alpha1 (0.01 2 2)
    );
    curls
    (
        U      (100 1e+05 3)
    );
    regions
    (
        cylinderToCell
        {
            minLevel 1;
            p1       (0.015 0.015 0.015);
            p2       (0.015 0.033 0.015);
            radius   0.006;
        }
    );
};
```

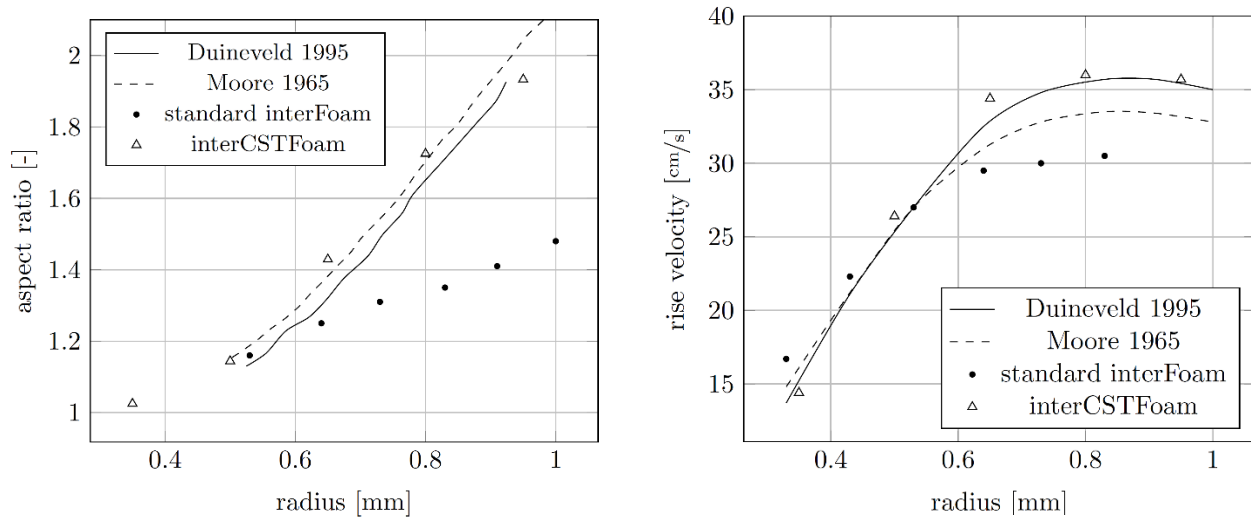
(b) Multi-refinement criterion dictionary

Figure 1: Concentration field around single rising bubbles.

Single Bubble Hydrodynamics

To be able to simulate rising single bubbles at higher Reynolds numbers, additional enhancements of the standard interFoam solver had to be undertaken. Utilizing the CICSAM scheme reduces numerical errors due to the discretization of the advection term compared to the standard MULES advection algorithm with additional bi-normal compression term. Further, the calculation of the surface tension force has been significantly improved by employing an iso-surface reconstruction of the interface to compute the interface normal vectors and including a smoothing algorithm for the resulting curvature. Validation of the improved solver framework is shown in Figure 2 by comparison of the bubble shape and bubble rise velocity against measurement results of [6] and [7]. It can be seen, that the numerical results of our

modified solver – compared to the standard interFoam solver – are in significantly better agreement to the experimental data.



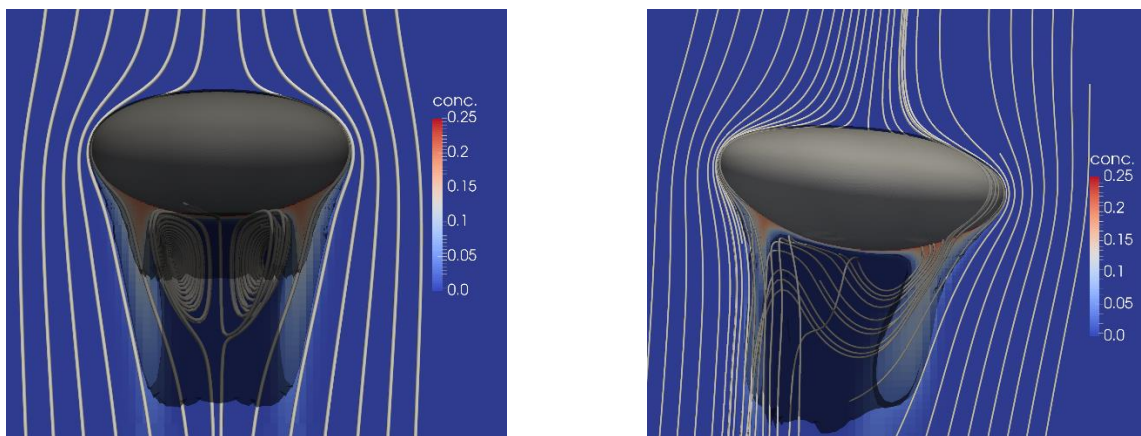
a) Bubble aspect ratio

b) Bubble rise velocity

Figure 2: Rising single bubble in ultra-pure water.

Interfacial Species Transfer

The main scientific aim of our research is the deduction of an improved interfacial species transfer correlation to be used e.g. in two-fluid models. Special focus lies herein in the investigation of the



a) $Eo=5$, $Mo=1e-05$ (ellipsoidal)

b) $Eo=0.3$, $Mo=1e-11$ (path instable)

Figure 3: Species concentration and velocity field.

influence of bubble shape and rise velocity onto the mass transfer at single rising bubbles. Especially the influence of bubble shape onto mass transfer processes has only briefly been discussed in literature so far, although it was found in this work to have a major impact due to the different resulting wake structures (see the difference in concentration wake structure depicted in Figure 3). Based on the enhanced hydrodynamic solver framework, an extensive parameter study has been conducted to derive an improved closure model for interfacial mass transfer from single rising bubbles. The resulting correlations for the interfacial area (here in terms of the surface ratio) and global Sherwood number are given in Figures 4a and 4b respectively. An interesting observation in Figure 4b is, that the decrease of the global Sherwood number as function of the bubble deformation seems to have a fixed lower bound.

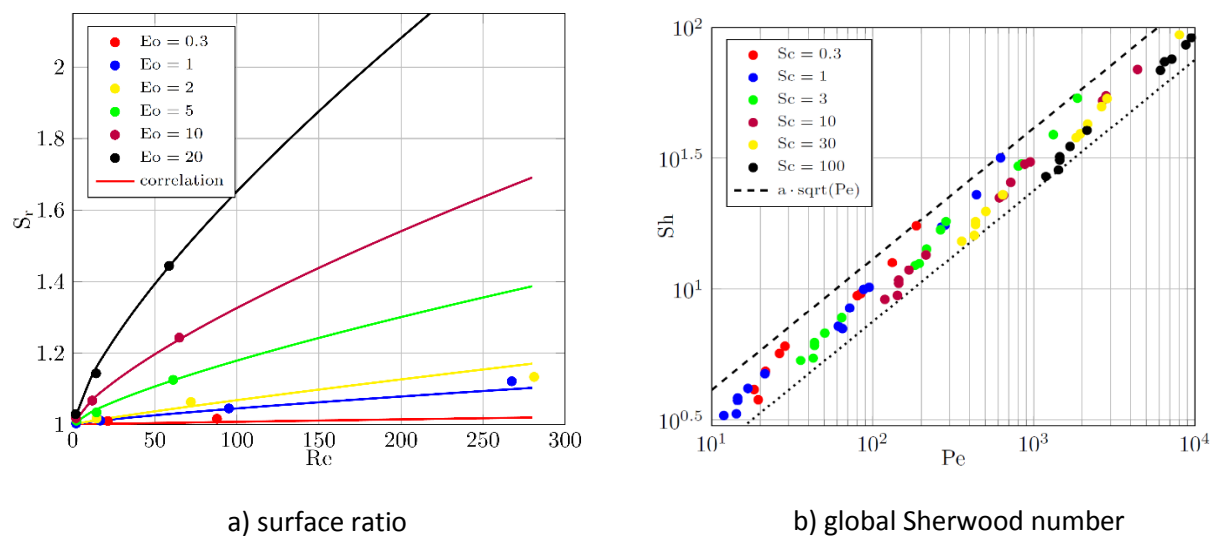


Figure 4: Mass transfer correlation for single rising bubbles - influence of bubble shape.

For strongly deformed bubbles, mass transfer is thus assumed to be mainly increasing due to the generation of additional interface. To additionally investigate chemical reactions, the species transfer library is coupled to the reaction library readily available within the OpenFOAM framework, allowing for the study of chemical reactions within the liquid phase. Recent development of the presented framework is dedicated to bounded implicit mesh-skewness correction methods to maintain accuracy and convergence order of the presented method also on strongly non-uniform meshes [3]. Also, a code release of the presented framework for the direct numerical simulation of species transfer in bubbly flows within the OpenFOAM-Extend project and OpenFOAM+ is planned for the near future. The source code related to local adaptive mesh refinement and dynamic load balancing is already available on the contributors branch of the ESI OpenFOAM+ repository.



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