Conf luenceS IMFT

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INSTITUT DE MECANIQUE DES FLUIDES

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Detailed modeling and simulation of mass transfer across fluid interfaces

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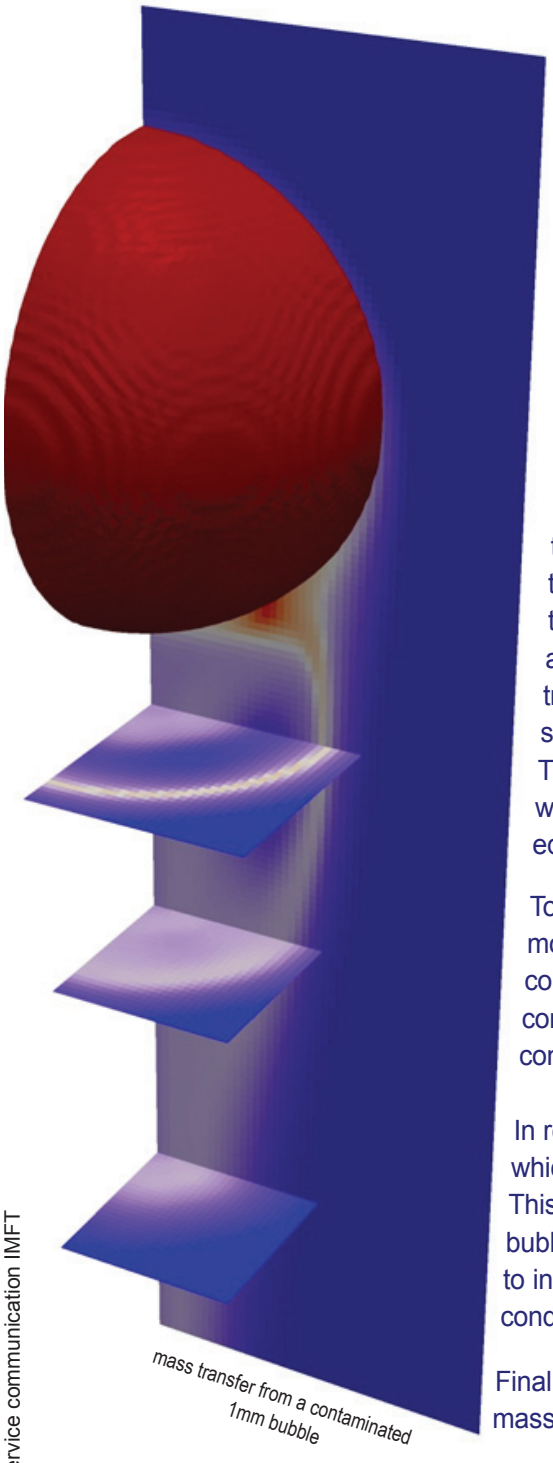

mass transfer from a contaminated 1mm bubble

Reactive mass transfer of, say, oxygen from rising gas bubbles to the ambient liquid is the basis for many chemical processes of industrial importance. Besides experimental investigations, the necessary intensification requires numerical simulations based on mathematical modeling. Our approach is based on continuum mechanical sharp-interface balances of mass, momentum and species mass. It employs the Volume of Fluid (VOF)-method to solve the two-phase Navier-Stokes equations with capillary interface, complemented by convection-diffusion-reaction equations for the involved chemical components.

The method uses two scalar variables for the concentration field of each transfer component, one for each phase. This allows for an intertwined treatment of the phase volume and molar species mass convection, employing the PLIC algorithm for the determination of the interface location. In this manner artificial mass transfer induced by numerical diffusion due to the convective transport step is avoided. Furthermore, the two-scalar approach enables a separate computation of the one-sided concentration limits at the interface. This is important for the calculation of the mass transfer across the interface which is modeled by an interchange term accounting for local thermodynamical equilibrium at the phase boundary.

To capture the thin concentration boundary layer at the bubble surface at least for moderate Reynolds and Schmidt numbers, the method is combined with several computational techniques. In particular, we employ a subgrid-scale model for the concentration profile, a moving window technique, and specific artificial boundary conditions to reduce the lateral computational domain size.

In real world applications, impurities and additives are present in the liquid phase which may adsorb at the bubble surface, modifying the surface tension locally. This leads to partially immobilized fluid interfaces which significant changes in the bubble hydrodynamics and mass transfer rates. We report on a novel approach to incorporate such effects into VOF-computations, using a modified transmission condition at the interface.

Finally, an outlook on recent extensions toward local volume effects and reactive mass transfer subgrid-scale modeling is given.

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