Modeling and simulation of mass-transfer across clean/contaminated fluid interfaces

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Mass transfer of gaseous components from rising bubbles to the ambient liquid is the basis for many chemical processes of industrial and technical importance. Besides experimental investigations, the necessary intensification requires numerical simulations based on detailed mathematical modeling. Our approach is based on continuum mechanical sharp-interface balances of mass, momentum and species mass. In this context, the standard model consists of the two-phase Navier-Stokes equations with constant surface tension, complemented by molar mass balances for all chemical components. While this is sufficient for dilute systems under certain additional assumptions, it is inappropriate for real world applications, where for instance volume effects are important or impurities and additives are present in the liquid phase which typically leads to partially immobilized fluid interfaces, significantly changing the bubble hydrodynamics and mass transfer rates. This talk reports on thermodynamically consistent model extensions which are required to capture this and other phenomena which occur due to the multi-physics of interfacial mass transfer. We also explain recent advances to incorporate such effects into detailed numerical simulations employing one of either the Volume of Fluid (VOF) method or the Interface Tracking method and discuss challenging open issues.