MULTI-SCALE SIMULATION OF TWO-PHASE AND THREE-PHASE FLOWS

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Dispersed multiphase flows with deformable interfaces are frequently encountered in industrial processes involving large scale synthesis of synthetic fuels and base chemicals. In addition to formation, coalescence and break-up of bubbles, mass and heat transfer in the presence of chemical transformations prevail. These complex processes significantly influence the specific interfacial area, mixing of chemical species as well as the large scale circulation patterns and ultimately the performance (conversion/selectivity) of multiphase chemical reactors.

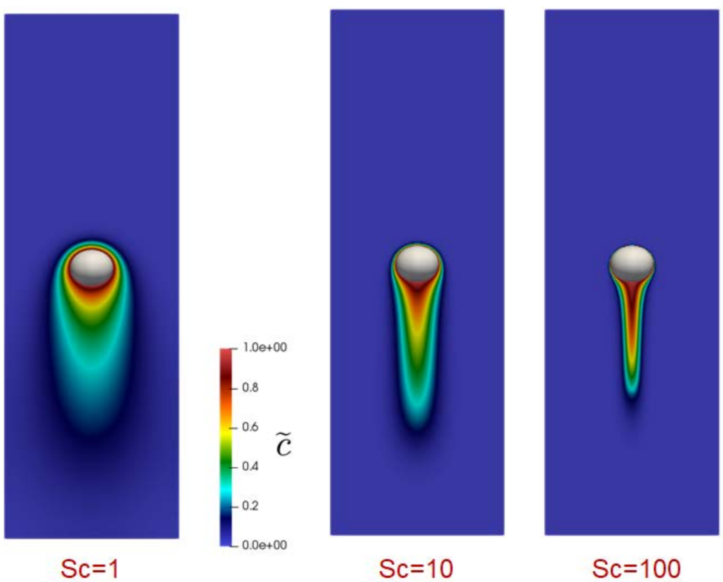

Figure 1: Mass transfer from a single rising bubble at several values of the Schmidt (Sc) number revealing considerable sharpening of the mass transfer boundary layer with increasing value of Sc.

For such complex flows involving mass, momentum and heat transfer a multi-scale modeling approach is adopted in which the interactions between the phases can be properly accounted for. The idea is essentially that detailed models are used to generate closures for the interphase mass, momentum and heat transfer coefficients to feed coarse-grained (such as stochastic Euler-Lagrange) models which can be used to compute the system behavior on a much larger (industrial) scale. In this contribution recent advances in the area of multi-scale simulation of dispersed two-phase and three-phase flows will be highlighted with emphasis on coupled mass, momentum and heat transfer. In addition, areas which need substantial further attention will be discussed.