DIRECT NUMERICAL SIMULATION OF FLUID INTERFACES INFLUENCED BY SOLUBLE SURFACTANT

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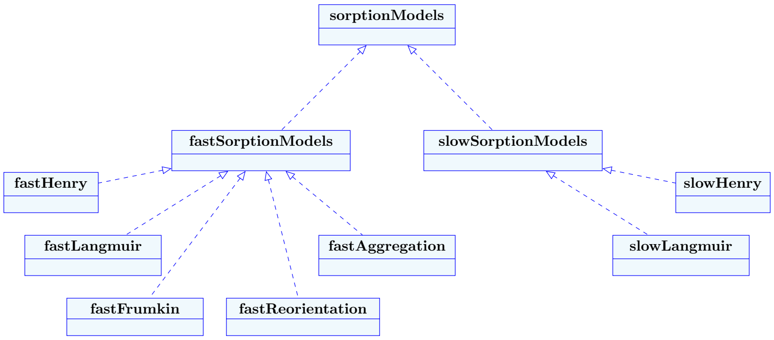
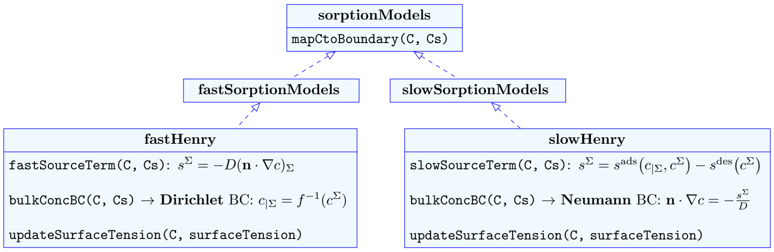
This study is concerned with continuum physical and numerical modeling of two-phase flows under the influence of surfactants. Surfactants are essential ingredients in many technological processes such as foaming or emulsification. Due to their amphiphilic character they accumulate at fluidic interfaces and modify the respective interfacial properties. Since these interfaces are moving and are continuously deformed and expanded, the local time-dependent interfacial coverage is the most relevant quantity. Direct Numerical Simulation (DNS) can give valuable insights into interfacial transport processes in such systems with surfactants, not easily accessible in experimental investigations.

The core part of the physical model consists in the description of the bulk and surface transport of surfactants with deformable interfaces, completed by proper boundary conditions and constitutive equations. In more details, when a surfactant solution comes in contact with a new surface, a transfer of molecules between the surface layer (free-surface or interface) and the layer immediately below it (sub-surface layer) occurs. Afterwards, there is an exchange of molecules between the sub-surface layer and the bulk phase, mostly due to diffusion. Within this process, two limiting adsorption regimes can be described: diffusion-controlled and kinetically-controlled adsorption. A *sorptionModel* library is implemented to describe these two sorption processes at the interface, cf. Fig.1. This implies a different treatment of the boundary conditions for the surfactant transport equations and the coupling between bulk and surface transport [1, 2].

The solution procedure is based on the Arbitrary Lagrangian-Eulerian (ALE) Interface-Tracking method, originally presented by Muzaferija and Perić [3] and extended by Tuković and Jasak [4]. Transport equations are solved using a collocated Finite Volume and Finite Area Method (FVM/FAM) on unstructured meshes of arbitrary topology with moving mesh support. The existing methodology was enhanced to describe a wider range of physical phenomena. A systematic study on mesh types and moving reference frame techniques is conducted to further investigate the solver stability.



(a) *sorptionModels*.



(b) *Example of sorptionModels functions*.

Figure 1: *sorptionModels* library structure.

The mathematical validation of the numerical method, mostly focusing on the sorption processes, cf. Fig.2, is performed by comparison against analytical solutions. Experimental results for single rising bubble in clean and contaminated water (e.g. Fdhila and Duineveld [5], Takagi et al. [6]) are compared to the simulation results to validate the overall numerical method. Such framework is then exploited to investigate the effects of surfactants on rising bubbles of different sizes and shapes, e.g. spherical bubbles and Taylor bubbles.

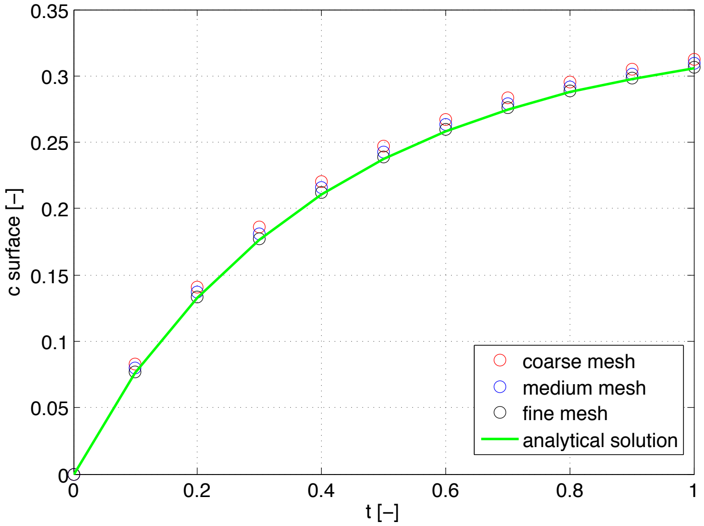


Figure 2: Validation of the sorption source term: surfactant concentration on the surface of a sphere due to *slow sorption* process from the bulk phase to the free surface.

The final aim is to investigate systems with surfactants being transported across the interface and diffusing in both phases via the process called partitioning [7], e.g. water/oil systems. In such case a two mesh approach is needed, since the physics to be described in the two phases require a separated treatment. Preliminary results regarding this approach will be presented.

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