

Modelling stagnant film mass transfer through mass transfer coefficient approach

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Stagnant film mass transfer between gas and liquid consisting of multiple species is commonly found in the industry, particularly for gasses absorbing into liquids. This study represents a novel industrial process comprising complex numerical simulations and experimental approaches. These mass transfer phenomena are comprehensively investigated using a computational fluid dynamics (CFD) approach with the Fluent software, where the interface is modelled through a volume of fluid (VOF) method. Volumetric source and sink terms are used to model the mass transfer, which are based on a mass transfer coefficient and the difference between the equilibrium density and actual density at the liquid side of the interface. These terms are included in the continuity and species transport equations. We also explore a similar model that considers the total resistance focusing on the gas side of the interface, using the difference between equilibrium partial pressure and actual partial pressure. The equilibrium conditions are found by carefully studying the phase diagrams of the system. To validate our CFD model, we compare the results with an approximate model solution, based on a lumped approach. The literature elucidation of the implementation of interfacial mass transfer using volumetric source and sink terms for VOF in Fluent is limited. Our findings indicate that mass conservation is achieved when special care is taken on the implementation of the source and sink terms.

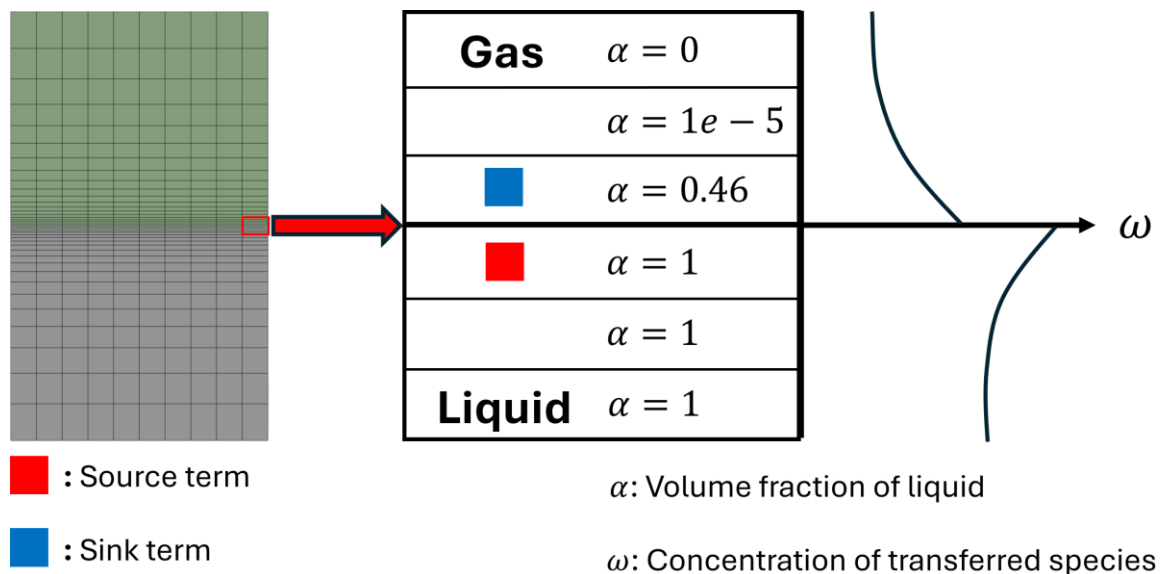


Figure 1: Numerical setup of case. Left: numerical grid refined close to interface. Centre: Possible configuration of source and sink terms and example values of volume fraction. Right: concentration profiles

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