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TOWARDS A MULTI-SCALE APPROACH FOR MULTI-PHASE CHANNEL FLOWS: SPECIAL BOUNDARY CONDITIONS FOR THE DIFFUSE INTERFACE MODEL

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When unit operations in process technology feature phase transition on large scales, a challenge for numerical simulations is their inherent multi-scale nature: bubble nucleation, coalescence, detachment from the wall, etc. The micro-scale phenomena influence heat transfer and fluid behavior on large scales. As it is numerically unaffordable to compute the whole system with a mesh capturing the micro effects, a multi-scale procedure is required: information computed on very fine grids capturing the interfacial regions is integrated in a simulation on coarser grids.

One of the novelties is the choice of the micro-scale model: the attractive features of the Diffuse Interface Model (DIM) are explored. This model captures the behavior of two phase flows with only one set of governing equations for both phases. In practice, the two phases are distinguished by plotting the value of the mass density: the low mass density regions correspond to the vapor phase while the high density areas represent the liquid. The governing equations are very similar to the conventional Navier-Stokes (NS) equations apart from the additional terms accounting for surface tension and the equation of state, which should be valid for both phases.

As the Diffuse Interface Model aims at solving the micro-scale situations arising from the macro-scale problem, one needs to develop special boundary conditions for the micro-scale that simulate the conditions experienced at the large scale: so-called open boundary conditions aim at simulating domains that appear to be infinite at the micro-scale and wall boundary conditions model the fluid and wall interactions.

Despite the active research in designing open boundary conditions for the NS equations, the extension to the DIM is complicated by the possible phase change at the edges of the computational domain and the treatment of the capillarity terms. The latter are responsible for imaginary characteristic speed that prevent application of the classical approach. A novel technique was developed in 1-D [1] and is here extended to 2D where the treatment of the transverse terms is now of major importance. This novel treatment of the boundary in combination with an extension of the wall interactions suggested by Jacqmin [2] and Spelt [3] enable the small scale simulation of bubble nucleation influenced by the inlet flow.

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