

Time-dependent Surface Properties of a Quaternary Mixture for an Esterification Reaction in Reactive Distillation

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In the process of designing and optimizing distillation columns, and reactive distillation, in particular, the knowledge of surface properties is indispensable. For instance, the catalytic surface in the inner of a packing column gets covered by the downwards-flowing liquid phase and is surrounded by the ascending vapor phase. The flow pattern and possible foam formation are determined by the surface properties. Apart from precise phase equilibria models, the surface tension in-between vapor and liquid is a crucial trait.

The time-dependent interface properties of reacting mixtures only have been calculated [1,2] regarding liquid-liquid interfaces using the NRTL model in combination with the density gradient theory (DGT) in its incompressible version [1]. The current approach is aiming towards describing the vapor-liquid surface of the esterification reaction 1-hexanol + acetic acid \rightleftharpoons water + hexyl acetate, based on the PC-SAFT equation of state [4] and the DGT in its compressible version [5]. For water, the approach suggested by Marshall [6], the so-called ARPC-SAFT, is applied. In contrast to PC-SAFT [5], the new approach [6] follows the associated reference perturbation theory, which incorporates the structural transition of water to tetrahedral symmetry. In the absence of water, ARPC-SAFT [6] is reduced to PC-SAFT [5].

This contribution discusses the performance of ARPC-SAFT together with DGT regarding the superposition of phase equilibria and reaction kinetics for this esterification reaction. For the first time, time-dependent surface properties (surface tension, density profiles, relative accumulation in the surface) are modeled for this reacting quaternary mixture.

References

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