A Systematic Modelling Framework for Phase Transfer Catalyst Systems

Phase-transfer catalyst systems contain two liquid phases, with a catalyst (PTC) that transfers between the phases, driving product formation in one phase and being regenerated in the other phase. Typically the reaction involves neutral species in an organic phase and regeneration involves ions in an aqueous phase. These reacting systems are receiving increased attention as novel organic synthesis options due to their flexible operation, higher product yields, and ability to avoid hazardous or expensive solvents. Major considerations in the design and analysis of PTC systems are physical and chemical equilibria, as well as kinetic mechanisms and rates. This paper presents a modelling framework for design and analysis of PTC systems that requires a minimum amount of experimental data to develop and employ the necessary thermodynamic and reaction models and embeds them into a reactor model for simulation. The application of the framework is made to two cases in order to highlight the performance and issues of activity coefficient models for predicting design and operation and the effects when different organic solvents are employed.

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