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Modeling and design of phase transfer catalytic processes

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A recent trend toward heterogeneous catalysis has been registered in the last decades. One of its most successful applications is represented by Phase Transfer Catalysis (PTC), which is now a mature technique for synthesis of organic chemicals from two reactants located in immiscible phases. In a PTC reaction, a phase transfer catalyst is added in order to transfer one of the reactants from its normal phase into a different phase where it can encounter and react with a second reactant which is immiscible with the first reactant's phase. Experimental studies have been the chief driving force behind most of the industrial applications in this area. Although extremely important, these studies are not, by themselves, adequate for efficient and optimal development of PTC reactions. To date, however, the engineering analyses needed to quantitatively complement an experimental program have been limited to a few studies on kinetic modeling of batch PTC reactions; relatively little is thus available in the form of a systematic approach to tackle conceptual process design problems. The objective of this study is to develop a systematic model-based framework that can be used for the design of PTC processes in conjunction with the insights obtained from experimental studies and the existing empirical knowledge. A coupled understanding of the interplay of kinetics, mass transfer, and thermodynamics, and their effects on the reactor performances will be provided. Challenging issues addressed in this study are the development of a reliable thermodynamic framework capable of predicting reactant and product concentrations in the two different phases, as well as the estimation of catalysts' physical parameters such as distribution coefficient and dissociation equilibrium constant. On the basis of these fundamental solubility data a systematic strategy for catalyst and solvent selection is proposed. Operating conditions are synthesized, analyzed, and evaluated on the basis of the reactive phase behavior. A case study is formulated to test the model and assess its predictive potential against experimental data.