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Reactive distillation column for the production of palm oil fatty acid ester: modeling and simulation

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In the present study, a post-design algorithm is applied for design of the reactive distillation column for production of isopropyl palmitate. In a reactive distillation column, the reaction and separation are implemented simultaneously within a single distillation column. The reaction is catalyzed heterogeneously by zinc acetate supported on functionalized silica. The developed kinetic model is presented. The algorithm makes extensive use of nonequilibrium (rate-based) simulation model. Thus, the reactive distillation process for the production of fatty acid ester from alcohol and fatty acid is simulated with the rate-based model RATEFRAC from the process simulator Aspen Plus (version 12.1). Experimental reaction kinetics data were incorporated into the process simulator. The UNIQUAC model was used for vapor-liquid equilibrium. The liquid-phase non-ideality was accounted in the model whereas the vapor phase was assumed to be ideal. Physicochemical properties such as phase equilibrium, liquid and vapor phase enthalpies were calculated utilizing the Aspen Plus software data-base. To ensure the most effective reactive distillation process, several key design parameters such as column pressure, reactive zone location, catalyst mass, reactant feed location, reflux ratio, column diameter, number of equilibrium stages and catalyst bed height were investigated by sensitivity analysis. The simulation study helped and resulted in the better design of reactive distillation column for the production of fatty esters.