Optimisation parameters of the reactive separations with very fast chemical reaction

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Abstract:

Reactive distillation is a merger of two key processes in the technology – production and separation – into one operation step. The complexity of such problem gives way to mathematical modelling.

In this work, steady-state model of non-equilibrium (NEQ) tray column is presented. Reaction system consists of four components taking part in two reactions one of which is very fast. The reactions are homogeneously catalysed so the reaction occurs also in the liquid film. Fick's equation was used to describe mass transfer in the liquid film, giving rise to a so-called reaction-diffusion equation. The other represents a boundary value problem (BVP) being second-order ordinary differential equation with boundary condition given in two points. Mathematical model then leads to a mixed system of strongly non-linear algebraic equations and second-order differential equations.

First the built non-equilibrium model had to undergo a benchmark with the equilibrium one. The comparison of production-prediction at two values of film thickness (representing various hydrodynamic conditions) between NEQ and EQ has been done. Modified Hatta number was used as an indicator of the processes taking place in the column.

The parameters that can be altered are number of trays, number and position of feeds, character of the feeds (from cool liquid to overheated vapour), composition of the feeds, reboiler capacity and duty, etc. This all, in combination with a reaction system that forms couple of azeotropes and hetheroazeotrope, creates a problem with multiple operating variables.

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