

Modeling and analysis of reactor-separator for equilibrium limited reversible reactions

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Highlights

- Severely equilibrium limited reversible reaction with volatile products is investigated
- Parametric sensitivity to understand the effect of thermodynamic and kinetic parameters
- Stripping is necessary for conversion but also plays a major role in enhancing selectivity
- Model validation by proof of concept experiments and strategy for selection of reactor

1. Introduction

There are several industrially relevant reversible reactions which are severely equilibrium limited yielding volatile products. For such reactions the in-situ removal of one or more products is necessary for the reaction to proceed. Several examples are given in literature e.g. Darda and Ranade (2012) [1] for Isophorone synthesis, Zhang et al. (2010) [2] for the synthesis of Dimethyl carbonate and Wang et al. (2014) [3] for the synthesis of Ethylene carbonate. If these volatile product species are highly soluble in the reaction media they must be stripped out from the reactor. For such a process there are many variables and design considerations. e.g. One can use different stripping agents, their flows and distribution/delivery into the reactor, the desired degree of removal of volatile products, operating conditions to favor efficient removal of products, number of stages, residence time requirements to get maximum selectivity and optimum conversion.

A limiting case would be where the main product forming reaction is second order liquid phase reactions which are slow and the byproduct reaction is of first order. For such slow liquid phase reactions, we would require liquid phase as continuous and gas as dispersed phase. In addition to it for volatile products where relative volatility is higher a CSTR type reactor with stripping/evaporation facility can be used as given in Schoenmakers and Bessling (2002) [4].

2. Methods

We have started with the mathematical model for one perfectly mixed stage reactor with product removal only through vapor phase. For model validation, some proof of concept experiments was conducted on a model one-stage reactor-separator system in laboratory. Depending on factors such as product formation rates and effective removal of them from the reactor (Damköhler numbers for reaction and mass transfer), the heat input contributing to evaporation rates, the holdup in reactor changes dynamically. The reactor contents may or may not be boiling depending on the operating conditions and liquid phase mole fractions. Learning from previous work such as dynamic model for gas-liquid reactor-separators by Ranade et al. (1999) [5] we have developed a mathematical model for reactor-stripper. Schematic diagram of the system under consideration is shown in Figure 1 (Left). Product outlet is in the form of vapor only whereas stripping agent may be an inert gas or superheated vapors or both. Key model equations are given here in brief. Eq. (1) and (2) give the component and overall mass balances for liquid phase in dispersion. Energy balance equations were written in line with mass balance equations.

$$\frac{d}{dt} [M_{i,n}^L] = \dot{m}_{n-1}^L z_{i,n-1}^L + \dot{m}_{n-1}^{AL} z_{i,n-1}^{AL} - \dot{m}_n^L x_{i,n}^L + \bar{R}_{i,n}^L V_n^D \varepsilon_n^L MW_i - \bar{N}_{i,n}^{LG} V_n^D MW_i \quad (1)$$

$$\frac{d}{dt}[M_n^L] = \dot{m}_{n-1}^L + \dot{m}_{n-1}^{AL} - \dot{m}_n^L - V_n^D \sum_{i=1}^c \bar{N}_{i,n}^{LG} MW_i \quad (2)$$

Eq. (3) and (4) describe component and overall mass balance for gas phase in dispersion.

$$\frac{d}{dt}[M_{i,n}^G] = \dot{m}_{n-1}^G z_{i,n-1}^G + \dot{m}_{n-1}^{AG} z_{i,n-1}^{AG} - \dot{m}_n^G y_{i,n}^G + V_n^D \bar{N}_{i,n}^{LG} MW_i \quad (3)$$

$$\frac{d}{dt}[M_n^G] = \dot{m}_{n-1}^G + \dot{m}_{n-1}^{AG} - \dot{m}_n^G + V_n^D \sum_{i=1}^c \bar{N}_{i,n}^{LG} MW_i \quad (4)$$

3. Results and discussion

At first the model and its solution was validated with proof of concept experiments. After model validation, numerical experiments were performed for various operating conditions. As shown in the right part of Figure 1, for different stripping rates (DaIII- Damkohler number for dimensionless mass transfer) with increase in the ratio of dimensionless reaction rate for desired to undesired reaction (DaI/DaII), conversion of limiting reactant drops but selectivity of the desired product increases continuously. In similar manner, findings are reported for parametric sensitivity with other key dimensionless parameters for inert gas, superheated vapor stripping and their combinations. Detailed results will be discussed in the full manuscript.

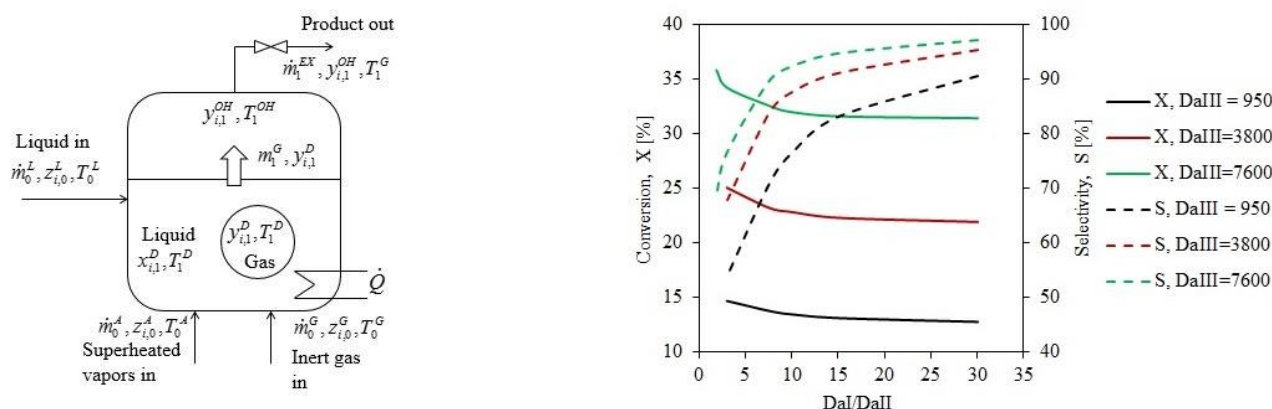


Figure 1. Reactor schematic (Left), Reactor performance (Conversion of limiting reactant and Selectivity of desired product) for stripping with superheated alcohol vapors (Right)

4. Conclusions

Model based analysis is performed to understand the dynamic behavior of a reactor-stripper with equilibrium limited desired reactions. Desired reactor performance necessitates the operation of reactor in region dominated by stripping which restricts the conversion of limiting reactant. Best performance was obtained with stripping by superheated vapors. Adequate stripping is not only necessary to get conversion but it also enhances selectivity of the desired reaction. These results will be useful in finalizing the appropriate reactor configuration and design.

References

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Keywords

“Reactive separation”, “Reactor modeling”, “Multiphase reactor”, “Process intensification”