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Dynamic investigation of high-purity/high-conversion generic reactive distillation

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Abstract

This paper presents the nonlinear dynamic analysis of an ideal two-reactant-two product reactive distillation. The impact of disturbance magnitudes and directions on openloop stability of the system is studied. An analysis of the physicochemical phenomena present in reactive distillation processes that, under certain operational conditions, causes special types of nonlinear behavior is carried. Operating two-reactant-two-product reactive distillation with excess of heavy reactant is found to enhance openloop stability, but decreases the products purity. However, excess of more volatile reactant drifts the system to another state. It is found that openloop reactive distillation system has a better dynamics when operated with fixing reflux ratio instead of reflux rate.

Keywords: Reactive distillation, nonlinear dynamic simulation, system stability

1. Introduction

The idea of combining reaction and separation in a single unit has been known for a long time with possible profitable applications. However, an incomplete understanding of the interactions of the many nonlinear phenomena like chemical reactions, phase equilibrium, mass transfer and countercurrent flow has limited a widespread use of such processes so far. In reactive distillation column especially with reactive section in between the rectifying and stripping section, the regions of intense mass transfer are in the reactive zone, while the ends of the column are essentially used for purification. Reactive region is more sensitive to disturbance directions as compared to the column ends. The effectiveness of disturbance suppression in a multivariable control system can depend strongly on the direction of disturbance (Skogestad & Morari, 1987). Thus, the potential advantages of reactive distillation could be negated by improper choice of reactant to be run in excess in the reactive zone whenever it is needed to avoid substiochiometry balance. It is possible to decrease conversion by increasing the amount of catalyst under certain circumstances (Higler *et al*, 1999). Increased separation capability could decrease process performance (Sneesby *et al*, 1998).

In this study, the openloop dynamic behavior of generic reactive distillation system is investigated. The main purpose is to analyze the impact of magnitudes and directions on

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dynamic stability of the system. Two openloop scenarios are explored: Fixed reflux rate and fixed reflux ratio.

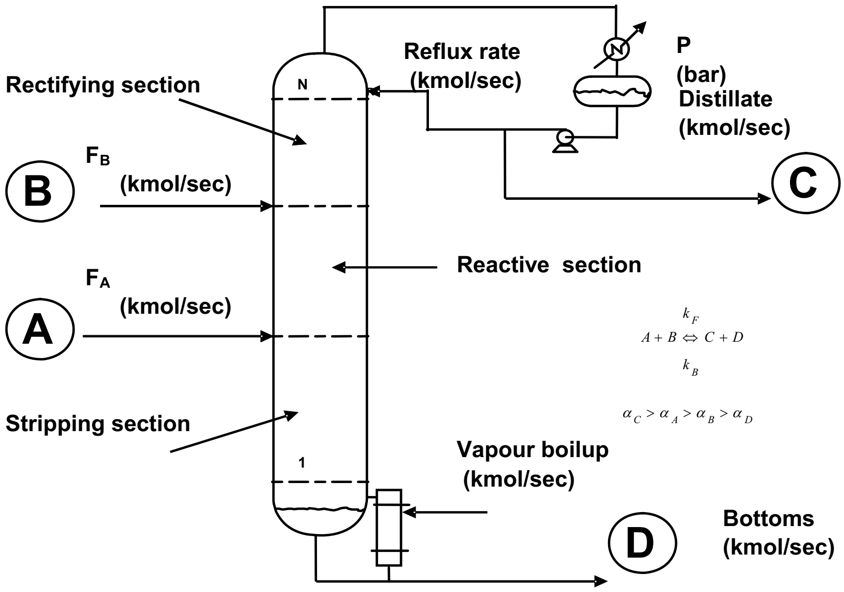


Figure 1. Distillation column

2. Process description

Among several chemical systems, two-reactant-two-product reactions have received wide application in reactive distillation technology (Sundmacher & Kienle, 2003). In this work, an ideal two-reactant-two-product reactive distillation is considered as shown in Figure 1. The column consists of 22 stages, including a total condenser, a partial reboiler, and 20 column stages. The main column is divided into three sections of which reactive zone (6 stages) is located in the middle with nonreactive rectifying and stripping sections (7 stages each) at the top and bottoms respectively. The column pressure is maintained at 9 bar. The reversible, exothermic liquid phase reaction occurs in reactive zone is $A + B \Leftrightarrow C + D$.

The task of the rectifying section is to recover reactant B from the product stream C. In the stripping section, the reactant A is stripped from the product stream D. In the reactive section the products are separated in situ, driving the equilibrium to the right and preventing any undesired side reactions between the reactants A (or B) with the product C (or D). The physical properties , kinetics , vapor-liquid equilibrium data and as well as the dynamic model for this process is given in Al-Arfaj & Luyben (2000). The base steady state conditions for this system are provided in Table 1.

3. Openloop dynamics

In order to investigate the dynamic behaviour of the system, the effect of disturbances with various magnitudes ranging from 1% to 10% in both positive and negative directions is studied. The process variables considered as sources of disturbances are the feed flowrate of reactant A (F_A), feed flowrate of reactant B (F_B) and vapor boilup (Vs).

Table 1. Base steady state conditions.

	Variables	Steady state conditions
Flowrates	Fresh feed of reactant A (kmol/s)	0.0126
	Fresh feed of reactant B (kmol/s)	0.0126
	Vapor boilup (kmol/s)	0.0285
	Reflux rate (kmol/s)	0.0331
	Distillate (kmol/s)	0.0126
	Bottoms (kmol/s)	0.0126
Composition in distillate	A	0.0467
	B	0.0033
	C	0.9501
	D	0.0000
Composition in bottoms	A	0.0009
	B	0.0445
	C	0.0000
	D	0.9545

The dynamics of the system under these changes were studied for two scenarios:

1. Openloop dynamics I (OL-I): reflux rate is fixed by changing reflux ratio and reflux drum level is controlled by distillate flowrate.
2. Openloop dynamics II (OL-II): reflux ratio is fixed by changing the reflux rate and reflux drum level is controlled by distillate flowrate.

In both scenarios, pressure is maintained by the heat removal from condenser while the base level is controlled by manipulating the bottoms flowrate.

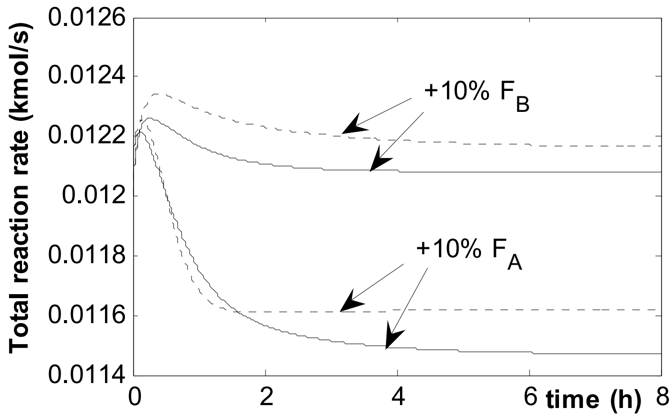
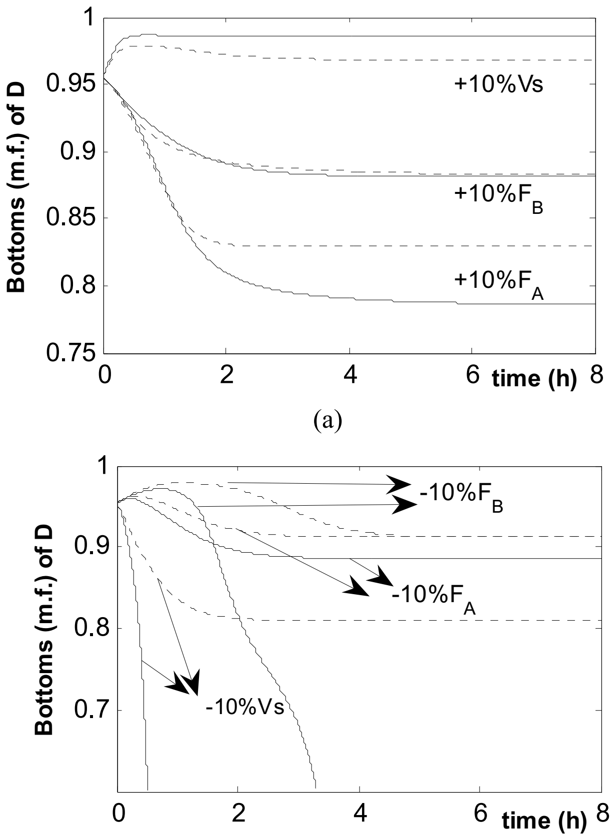


Figure 2. Dynamic responses of total reaction rate to positive step changes in feed fluorites of reactant A and B. (—) OL-I; (---) OL-II.

4. Results and Discussion

The impact of disturbances from feed flowrates in the kinetic region of reactive distillation is first explored. Figure 2 compares the total reaction rate responses in the reactive zone for the two scenarios when a 10% increase in feed flowrates is introduced. As can be seen, there is no much difference in the responses of OL-I and OL-II. The result shows that operating the system with excess of reactant B, the heavy reactant, in the reactive zones slightly increases the total rate of reaction. This is primarily due to the fact that reactant B will concentrate more in the liquid phase and will react with the available reactant A whenever it is available in excess. On the other hand, excess of reactant A in the column drifts the system sharply to another state and results in fast decrease in total reaction rate.

Even though increasing the fresh feed of reactant B has the advantage of increasing the conversion and enhancing the system stability, yet it decreases products purity as shown in Figure 3a. This will always be the case irrespective of which scenario is employed.



(a)

(b)

Figure 3. Composition dynamic responses of product D in bottoms to step changes in feed flowrate of reactant A (F_A), feed flowrate of B (F_B) and vapor boilup (Vs). (—) OL-I; (---) OL-II.

Figure 4 shows the effect of negative disturbances in feed flowrate of reactant B (F_B) for the two scenarios studied. Introducing a negative disturbance in F_B has a severe impact on the dynamics of the system, and consequently its stability when reflux rate is fixed (OL-I) instead of reflux ratio. Reducing F_B by 2% drifts the system to another state. Further decrease in feed flowrate F_B will result in an unstable operation. The rapid build-up of the reactant A concentration in the reactive zone decreases the system stability because an excess of a more volatile reactant A will demand either an increase in heat duty of the system (which is fixed in this case) in order to strip out any unreacted A from product D or a decrease in reflux rate to reduce the amount of reactant A returning into the system. On the other hand, a decrease in feed flowrate of reactant B when reflux ratio is fixed (OL-II) will only drift the system into a lower state as shown in Figure 3.

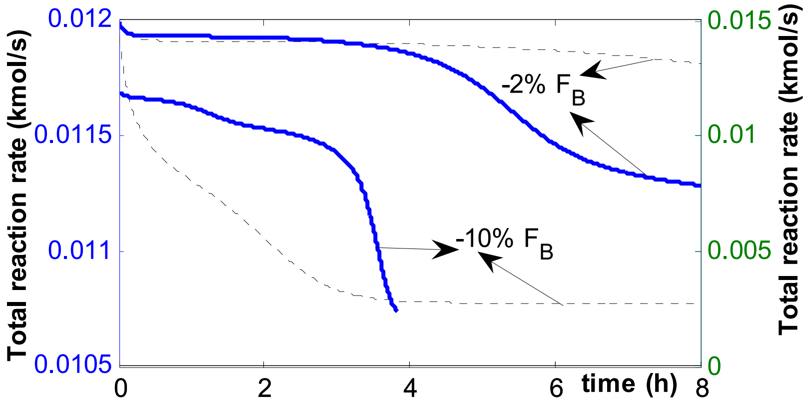


Figure 4. Dynamic responses of total reaction rate to negative step changes in feed flowrates of reactant A and B. (—) OL-I; (---) OL-II.

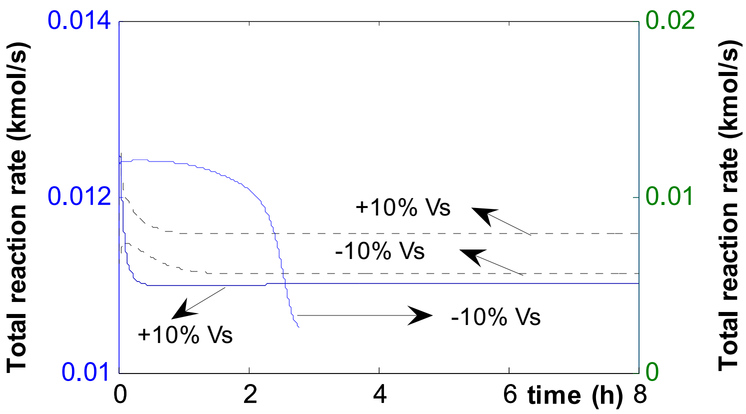


Figure 5. Dynamic responses of total reaction rate to step changes in vapor boilup (Vs) (—) OL-I; (---) OL-II.

Figure 5 compares the dynamic response of the total reaction rate in the reactive zone for the two scenarios (OL-I and OL-II) after step changes of ±10% in vapor boilup are made. Changing the vapor boilup alters the fractionation capacity of the column. As vapor rate from the reboiler increases, more heat will be available to enrich volatile components in vapor phase than needed, thus causing stochiometirc imbalance of the reactants in reactive zone because liquid concentration of reactant A is reduced. This results in decrease total reaction rate as shown in Figure 5. This reduction in the rate of product formation in the reactive zone is significant in OL-I scenario because more of reactant A is lost in the overhead when reflux rate is fixed. Decreasing the vapor boilup from its base steady state value makes the system unstable (see Figure 5) when reflux rate is fixed. The purity of bottoms decreases rapidly because of the presence of more than expected reactants in the stripping section (see Figure 3b). This is due to the interference effect of fractionation on the system's reaction kinetics, which will require change in reflux rate for necessary compensation.

Generally, openloop dynamics of reactive distillation will give a better performance when the reflux ratio is fixed instead of reflux rate. However, if fixing the reflux rate is preferable or needed, the inclusion of internal inventory composition controller and/or single end controller (composition or temperature) are expected to resolve most of the instability problems.

Conclusion

The impact of disturbance magnitudes and directions on the dynamic stability of reactive distillation system has been investigated. This study demonstrates that openloop reactive distillation system gives a better performance when operated with fixing reflux ratio instead of reflux rate. Excess of less volatile reactant in two-reactant-two-product generic reactive distillation is found to enhance openloop stability, but decreases the products purity. On the other hand, excess of more volatile reactant triggers the system to another state.

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