

Comparison of Alternative Control Structures for an Ideal Two-Product Reactive Distillation Column

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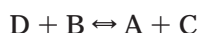
Although steady-state design and open-loop dynamics of reactive distillation columns have been explored in many papers, very few papers have dealt with closed-loop control. Most of these control papers consider reactive distillation columns in which there is only one product, and an excess of one of the reactants is sometimes assumed. This paper explores the closed-loop control of a reactive distillation column in which two products are produced in a single column and stoichiometric amounts of fresh feeds are desired. The reversible reaction is $A + B \rightleftharpoons C + D$. The relative volatilities are favorable for reactive distillation; i.e., the reactants are intermediate boilers between the light product C and the heavy product D. Simple ideal physical properties, kinetics, and vapor–liquid equilibrium are assumed so that the basic control issues of reactive distillation can be explored without being clouded by complexities of a specific chemical system. Six alternative control structures are evaluated via rigorous dynamic simulation. All of the schemes use a composition analyzer in the reactive zone of the column to detect the inventory of one of the reactants so that fresh feed can be manipulated to satisfy the reaction stoichiometry. Therefore, the use of excess reactant is not required. The interaction between design and control is illustrated by the impact of holdup in the reactive zone: increasing holdup (catalyst) improves the dynamic controllability of the process. Single-end temperature control can keep both products at or above specified purity values, even for large disturbances, if reactive-zone holdup is sufficiently large.

1. Introduction

Reactive distillation has been employed in industry for many decades, but its area of application has grown significantly in the past decade. Reactive distillation can reduce capital and energy costs in some systems, particularly when reactions are reversible or when the presence of azeotropes makes conventional separation systems complex and expensive. Of course, the reaction temperatures must be suitable for vapor and liquid phases to exist, and the volatilities of the reactants and products must be such that the products can be removed while containing the reactants in the column.

Many papers have analyzed reactive distillation columns under steady-state conditions. The literature up to 1992 was reviewed by Doherty and Buzad.¹ Since that time, several papers considering steady-state design and optimization have appeared.^{2–6} Several papers have studied the open-loop dynamics of reactive distillation,^{7–12} with most of the interest in multiple steady states. Only a handful of papers^{13–19} have appeared that discuss the closed-loop control of reactive distillation columns.

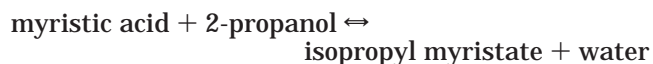
In one of the earliest control papers, Roat et al.¹³ studied a two-product reactive distillation column with the reaction



where the control objective was to control the purity of the distillate product (mostly A) and conversion. They proposed a control structure that used two conventional proportional–integral (PI) temperature controllers to

maintain two tray temperatures in the column by adjusting the two fresh feed streams. The reflux ratio and vapor boilup were held constant. Production rate changes were achieved by changing the vapor boilup. The scheme could handle 5% increases in throughput. In our paper we will subject the column to much larger disturbances and have specifications on both product purities.

Bock et al.¹⁴ proposed a control scheme for a coupled two-column reactive distillation process that is reported to control the purities of both of the products. The esterification reaction considered is



Fresh acid, fresh 2-propanol, and a 2-propanol/water recycle are fed to the first column (a reactive stripper). The heavy ester product is taken out of the bottom. The water product goes overhead with some isopropyl alcohol (IPA) because IPA and water form an azeotrope. This overhead stream is fed to a second nonreactive column in which the water product is taken out of the bottom and the overhead vapor, which has a composition close to the IPA/water azeotrope, is fed back to the reactive stripper. The proposed control scheme looks reasonable except for the use of a simple ratio scheme to balance the reaction stoichiometry: fresh 2-propanol feed is simply ratioed to fresh acid feed. In computer simulations, this scheme may work, but its effectiveness in a plant environment is questionable. There is always some significant inaccuracy in flow measurements, and even the slightest imbalance between the moles of acid fed and the moles of IPA fed would lead to a gradual buildup of the component that is in slight excess because there is no way for the reactants to leave the closed

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system except through reaction. Some type of feedback of the inventory of at least one of the reactants in the system is required.²⁰

Kumar and Daoutidis¹⁵ studied the control of a reactive distillation column in which ethylene oxide and water react to form ethylene glycol. A consecutive reaction to form diethylene glycol also occurs. Fresh ethylene oxide and fresh water are fed into the column, and the product is removed from the base. There is no distillate product. The variables the authors chose to control are pressure, base level, and the purity of the bottoms product (the concentration of ethylene glycol). The paper does not say how the fresh feed streams are introduced, so we can infer that they are both simply flow controlled. This structure would suffer from the same problem of stoichiometric imbalance discussed in the previous paragraph. The author studied an input/output linearizing controller that was claimed to be effective at moderate product purities but was unstable at higher purities. The authors also tried conventional PI controllers but claim that a more advanced nonlinear controller is needed.

In a recent paper, Vora and Daoutidis¹⁶ extend this work to the ethyl acetate reactive distillation case. Although there are both distillate and bottoms products in this column, they only control the distillate purity. They again use a nonlinear input/output linearizing state feedback controller, which is tested by making setpoint changes in the distillate composition controller. The two fresh feed streams are apparently flow controlled, so the proposed structure suffers from the stoichiometric imbalance problem.

Sneesby et al.¹⁷ proposed a two-point control scheme for an ethyl *tert*-butyl ether (ETBE) reactive distillation column in which both bottoms product purity and conversion are controlled. Conventional PI controllers are used to control a temperature in the stripping section by manipulating the reboiler heat input and to control conversion by manipulating the reflux flow rate. Conversion is calculated inferentially from several temperature and flow measurements.

Bartlett and Wahnschafft¹⁸ studied the control of a methyl *tert*-butyl ether (MTBE) reactive distillation column. Several schemes using conventional PI controllers are discussed. The selection of an appropriate tray temperature is explored. They recommend the use of a tray in the reactive section instead of the more conventional approach of using a temperature in the stripping section. The authors recognized the importance of maintaining tight control over the feed stoichiometry to avoid an excess of methanol. They first tried to measure the methanol concentration in the overhead and manipulate methanol fresh feed, but found that there was severe interaction between the temperature controller and the methanol composition controller. They finally recommended a feedforward scheme in which the feed composition is measured and used to reset the fresh methanol feed flow rate. The flaw in this type of open-loop ratio approach has already been discussed above. Flow measurement inaccuracies and composition analyzer inaccuracies would doom this strategy to failure in a real plant environment unless significant amounts of excess methanol are used.

Balasubramhanya and Doyle¹⁹ recently applied nonlinear model-based control to a batch reactive distillation column producing ethyl acetate. We do not consider batch reactive distillation in this paper.

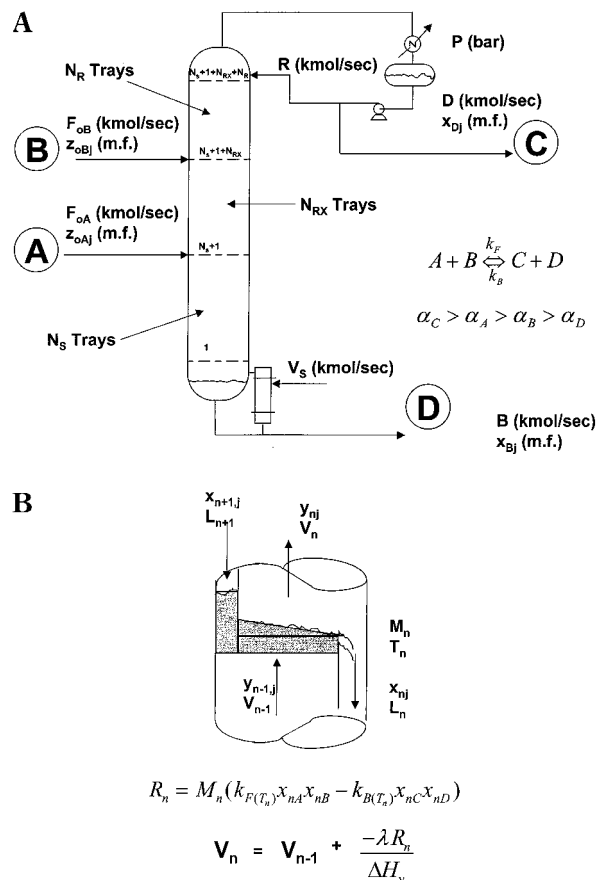


Figure 1. (A) Ideal reactive distillation column. (B) Reactive tray.

Most of the control studies discussed above deal with real chemical systems. While this provides the flavor of reality to the studies, it imposes severe constraints on the conclusions to be drawn. Each system has its own set of complexities in vapor–liquid equilibrium nonideality (azeotropes), reaction kinetics, physical properties, etc. Simulations of these complex systems are also subject to considerable uncertainty because different commercial simulators frequently give greatly different results when presumably using the same physical property packages and kinetics. This problem has been addressed in several papers; one recent example is Whiting and Xin.²¹ These comments are not intended as criticism of previous work. Certainly the study of real systems is vital. However, we feel that it might be useful to first attack a more simple problem and see what basic insights can be gained.

In this paper we do not want to cloud the picture with the specific complexities that are typical of many real chemical systems. We want to study an ideal generic reactive distillation process with simple vapor–liquid equilibrium, simple reaction kinetics, and simple physical properties. Therefore, we strip away all of the complexities of nonideal behavior and consider a system with constant relative volatilities, equimolar overflow, fixed heat of reaction and heat of vaporization, saturated liquid feed and reflux, and constant pressure. This system can be used by process control researchers who wish to compare their results with those of others without any problems with differences in simulator software packages. The dynamic model of this simple system is presented below and can be easily programmed. Copies of a FORTRAN program are available from the authors.

Table 1. Physical Properties^a

activation energy (cal/mol)	forward	30 000			
	backward	40 000			
specific reaction rate at 366 K (kmol·s ⁻¹ ·kmol ⁻¹)	forward	0.008			
	backward	0.004			
heat of reaction (cal/mol)		-10 000			
heat of vaporization (cal/mol)		6944			
relative volatilities	α _C	8			
	α _A	4			
	α _B	2			
	α _D	1			
		C	A	B	D
vapor pressure constants	A _{VP}	13.04	12.34	11.45	10.96
	B _{VP}	3862	3862	3862	3862

^a $\ln P_j^s = A_{VP,j} - B_{VP,j}/T$ where T is in degrees Kelvin and P_j^s is the vapor pressure of pure component j in bar.

2. Process Studied

Let us consider the classical reactive distillation column shown in Figure 1. The reversible reaction occurring on the reactive trays is



The volatilities are such that the products C and D are the lightest and heaviest, respectively, in the system.

$$\alpha_C > \alpha_A > \alpha_B > \alpha_D \quad (2)$$

The reactants A and B are intermediate boiling between the products. Therefore, the fresh feed stream F_{OA} containing reactant A is fed at the bottom of the reactive zone, and the fresh feed stream F_{OB} containing reactant B is fed at the top of the reactive zone. The reactive section contains N_{RX} trays. The rectifying section above the reactive section contains N_R trays, and the stripping section below the reactive section contains N_S trays. Thus, we are considering a reactive distillation column in which reaction only occurs in the reactive section. This is typically the situation when the reaction uses a solid catalyst that is present on the trays in the reactive section. This type of reactive distillation is called catalytic distillation or recently has been called a "hybrid" system.¹² When we talk about changing tray holdup, this implies changing the amount of catalyst. The units and nomenclature used are illustrated in Figure 1A.

The forward and backward specific reaction rates (kmol·s⁻¹·kmol⁻¹) on tray n are given by

$$k_{Fn} = a_F e^{-E_F/RT_n} \quad (3)$$

$$k_{Bn} = a_B e^{-E_B/RT_n} \quad (4)$$

where a_F and a_B are the preexponential factors, E_F and E_B are the activation energies, and T_n is the absolute temperature on tray n . Table 1 gives kinetic and physical property data for the system. The net reaction rate for the production of C (kmol/s) on tray n in the reactive zone is given by

$$\mathcal{R}_{Cn} = M_n(k_{Fn}x_{nA}x_{nB} - k_{Bn}x_{nC}x_{nD}) \quad (5)$$

where M_n is the liquid holdup on the tray. If catalytic

Table 2. Base-Case Conditions; Ideal System

flow rate (kmol/s)					
fresh feed F_{OA}		0.01260			
fresh feed F_{OB}		0.01260			
reflux		0.03712			
vapor boilup		0.03248			
top tray vapor		0.04971			
distillate		0.01260			
bottoms		0.01260			
pressure (bar)		5.1			
tray holdup (kmol)		1.00			
tray number					
stripping		10			
reactive		10			
rectifying		10			
temperature (K)					
base		411.8			
top stripping		379.8			
top reactive		369.9			
top rectifying		340.0			
		A	B	C	D
composition (mole fraction)					
distillate		0.04985	0.00025	0.94989	0.00000
bottoms		0.00015	0.04983	0.00000	0.95003

distillation is considered, the weight of the catalyst on the tray would be used. See Figure 1B.

The dynamic component balance on tray n for product C is

$$\frac{d(x_{nC}M_n)}{dt} = L_{n+1}x_{n+1,C} + V_{n-1}y_{n-1,C} + \mathcal{R}_{Cn} - L_nx_{nC} - V_ny_{nC} \quad (6)$$

Similar balances apply for the other three components with the appropriate sign for the reaction rate term. Vapor holdup and pressure drop are neglected. Liquid hydraulics are included by using a linearized form of the Francis Weir formula with a 6 s hydraulic time constant.

The vapor-liquid equilibrium is assumed to be ideal. See Table 2 for vapor pressure data.

$$P = x_{nA}P_{A(Tn)}^s + x_{nB}P_{B(Tn)}^s + x_{nC}P_{C(Tn)}^s + x_{nD}P_{D(Tn)}^s \quad (7)$$

where total pressure P and vapor pressures P^s are in bar. The column pressure is fixed at 5.1 bar because this gives a reflux-drum temperature high enough to permit the use of cooling water in the condenser.

Because equimolar overflow is assumed, the steady-state vapor and liquid rates are constant through the stripping and rectifying sections. However, these rates change from tray to tray in the reactive zone because the heat of reaction vaporizes some liquid on each tray (see Figure 1B).

$$V_n = V_{n-1} - \mathcal{R}_{Cn}\lambda/\Delta H_v \quad (8)$$

$$\frac{dM_n}{dt} = L_{n+1} - L_n + \mathcal{R}_{Cn}\lambda/\Delta H_v \quad (9)$$

where λ is the heat of reaction (-10 000 cal/mol) and ΔH_v is the latent heat of vaporization (6944 cal/mol). There is an increase in the vapor flow rate up through the reactive zone and a corresponding decrease in the liquid flow rate.

The steady-state conditions are given in Table 2. The two fresh feed flow rates are each 0.0126 kmol/s of pure reactants. Conversion is 95%. Remember that essentially all of C leaves in the distillate and all of D

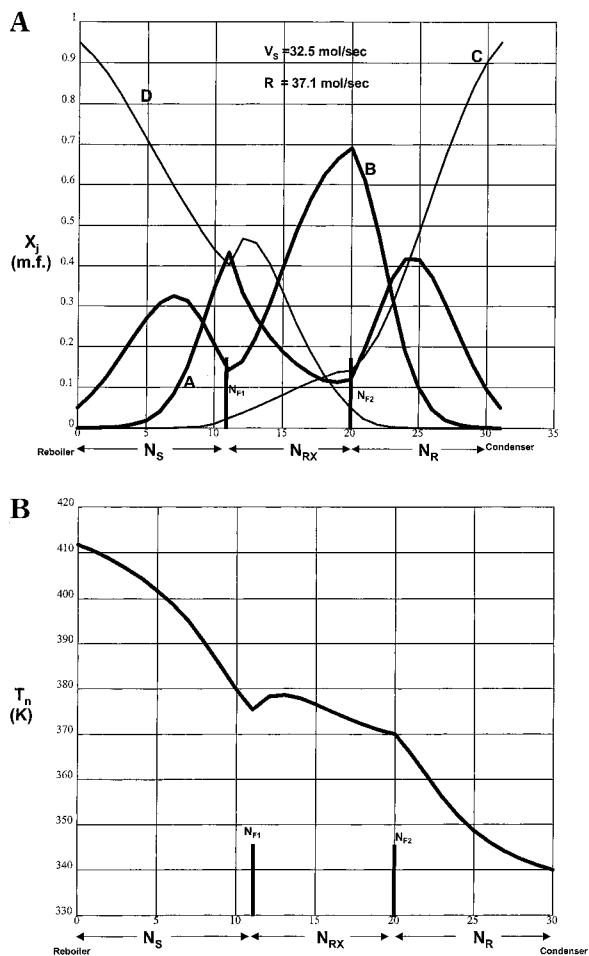


Figure 2. (A) Composition profiles. (B) Temperature profile.

leaves in the bottoms because of the relative volatilities. The reflux ratio is about 3, so it is reasonable to use either distillate or reflux flow rate to control the reflux-drum level.

Figure 2A gives the steady-state composition profiles for all four components. Note that reactants A and B have fairly high concentrations in the reactive zone but are prevented from leaving the top or bottom of the column by the rectifying and stripping trays. The principal impurity in the bottom is B, and that in the top is A. However, either reactant can be lost out of both ends if it is not consumed in the reactive zone. Figure 2B shows the steady-state temperature profile. There is a fairly significant temperature break around tray 5, and this tray temperature will be used in one of the control schemes to infer bottoms purity. The same is true for tray 25 near the top of the column. It could be used to infer distillate purity. In this paper we look at the use of just one tray temperature, but research is in progress for looking at the use of multiple temperatures.

3. Control Structures

In many practical applications it may be necessary to use temperature measurements instead of composition measurements. However, in this study we do not want to restrict ourselves to just temperature measurements because we explore a wide variety of control structures in order to see the full potential of the system. Therefore, we assume that we can measure any composition we need. Six alternative control structures are

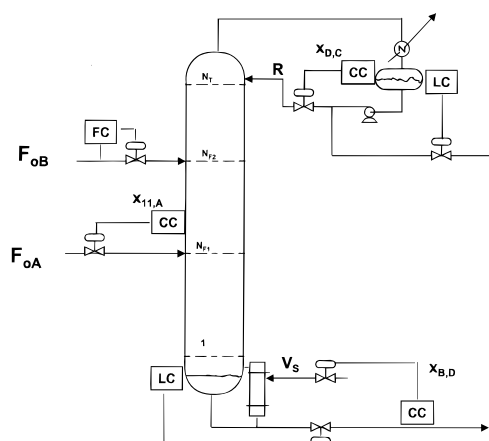


Figure 3. Control structure CS1; control purities.

discussed in the following sections. In all of these control schemes, the following loops are used:

1. Pressure is controlled by condenser heat removal.
2. The base level is controlled by manipulating the bottoms flow rate.

3. The concentration of reactant A on tray 11 at the bottom of the reactive section is measured and controlled by manipulating the fresh feed flow rate of component A (F_{oA}).

This last loop is perhaps the most controversial aspect of this paper. It requires a composition analyzer so that the inventory of component A in the system can be detected and feedback can be used to prevent the gradual buildup or depletion of one of the reactants. The process acts almost like a pure integrator with respect to the reactants. Only small amounts of the reactants are lost in the product streams. Exactly 1 mol of A is required for each 1 mol of B fed. Therefore, some feedback of information about reactant inventory inside the system is required for an effective control system.²⁰

One alternative to using this composition analyzer is to use a slight excess of one of the reactants. This excess has to be sufficient to handle the worst-case changes in feed compositions and flow-measurement inaccuracies. The latter can be quite large (10–20%) in many real plants. The excess reactant would remain in one of the product streams, and this stream would have to be further processed to purify the product and recover the reactant for recycle. This implies increased capital and operating costs.

Therefore, in this paper we chose to examine a stoichiometrically balanced fresh feed situation in which an analyzer is used. It is recognized that on-line analyzers are usually expensive and sometimes unreliable, but some type of feedback information is needed if we want to run a “neat” process (stoichiometrically balanced fresh feeds). It may be possible in some systems to infer this composition by using multiple temperatures and state estimation, but this is left for a future paper.

The issue of analyzer accuracy also needs to be addressed. Any drifting of composition signals could cause problems, but the absolute accuracy of the analyzer should not be a problem because the absolute level of the analyzer signal can be adjusted from steady-state performance data. What matters is analyzer sensitivity; the analyzer must detect changes in compositions. Even an inaccurate analyzer would prevent the stoichiometric feed problem because the change in its signal will indicate the buildup or depletion of the component.

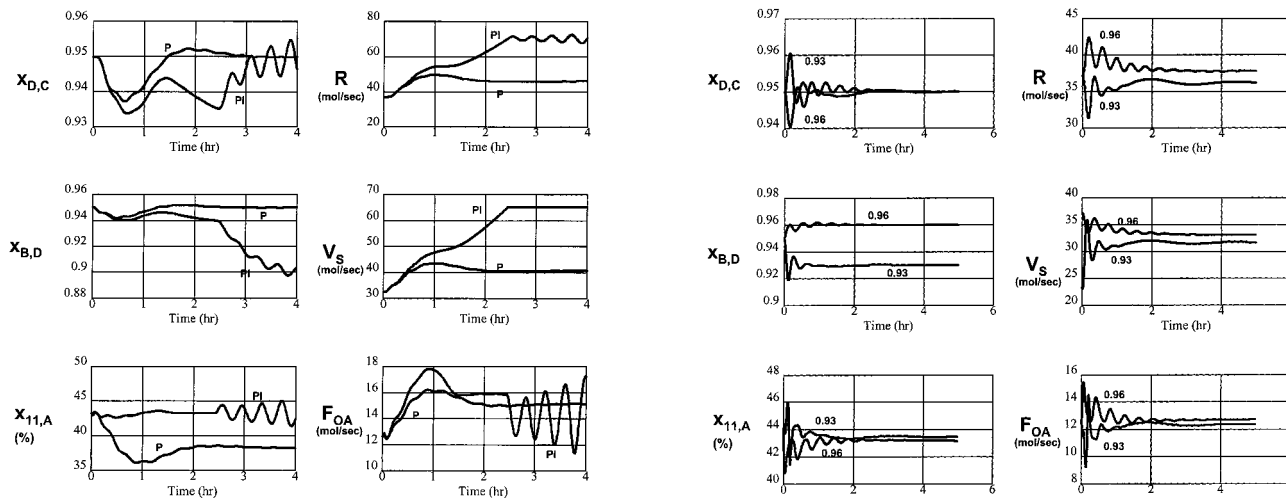


Figure 4. CS1; +20% F_{OB} ; P and PI for $x_{11,A}$.

Tray 11 was selected on purely heuristic grounds: this is where the concentration of A is the highest. Whether this is the best location is an open question and will be the subject of future study. We chose to measure the A composition and manipulate the fresh feed of A (F_{OA}). However, the alternative of measuring the internal composition of B and manipulating F_{OB} should be a viable alternative. We did not study this configuration.

3.1. Control Structure CS1. Figure 3 shows a control scheme CS1 in which the purities of both products are measured and controlled. In the distillate product, the composition of component C is controlled by manipulating the reflux flow rate. In the bottoms, the composition of component D is controlled by manipulating the vapor boilup. The fresh feed F_{OB} is the production-rate handle and is flow controlled. The reflux-drum level is controlled by the distillate flow rate.

Proportional-only level controllers are used. Composition controllers are PI with measurement lags (two first-order lags of 30 s each). These loops are tuned by conducting relay-feedback tests to find ultimate gains and frequencies and then using the Tyreus–Luyben settings. All control valves are designed to be half open at the initial steady state. Therefore, all manipulated variables cannot increase more than twice their steady-state values.

Figure 4 compares the use of PI and P controllers on the $x_{11,A}$ – F_{OA} loop. The disturbance is a 20% increase in the F_{OB} fresh feed flow rate. Trying to hold a constant composition of A on tray 11 with the PI controller drives the vapor boilup to its limit after about 2 h and leads to instability. The P controller lets the composition float to a new lower steady-state value, and the system handles the disturbance well. A controller gain of 2.5 is used in the P controller with a composition transmitter span of 50%. The Tyreus–Luyben tuning constants used in the PI controller are $K_c = 5$ and $\tau_I = 3.3$ min. It may be possible to retune the PI controller and achieve stable operation, but this was not studied because the P controller is simpler and works well. Because the column acts as a pure integrator with respect to reactant compositions, the use of a PI controller would be expected to present a tuning problem because the loop has two integrators in series.

Figure 5 shows the response of the closed-loop system for setpoint changes in the desired purity of the bottoms product from its base-case value of 95%. Figure 5A

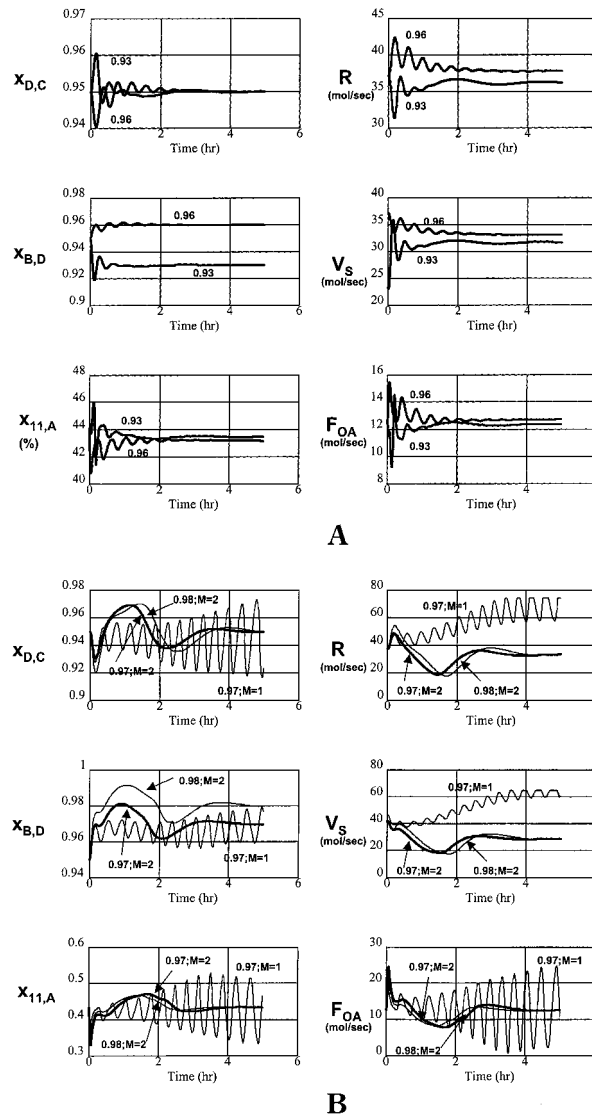


Figure 5. (A) CS1; $x_{B,D}$ changed to 0.93 and 0.96. (B) CS1; $x_{B,D} = 0.97$ ($M = 1$ and 2); $x_{B,D} = 0.98$ ($M = 2$).

shows that decreasing the purity to 93% or increasing the purity slightly to 96% can be handled. However, Figure 5B shows that a slightly higher setpoint of 97% cannot be handled, and the system becomes unstable. The fundamental problem is not the control structure but the fact that the reactive zone in the column does not provide enough holdup time (catalyst) to achieve the conversion required by this higher product-purity specification.

When the holdup in the column is increased from the base case 1 kmol/tray to 2 kmol/tray, as shown in Figure 5B, quite large setpoint changes can be easily handled (at least up to 98%). In these runs the initial conditions for all compositions and flow rates are those corresponding to the base case 1 kmol/tray holdup. At time equal to zero, the disturbance is made and the tray holdups are changed. A more rigorous approach would be to use the new steady-state conditions that correspond to the higher holdup and then introduce the disturbance. However, the final steady-state conditions would be the same, assuming the system does not exhibit closed-loop multiple steady states.

These results illustrate an extremely important point: providing plenty of reaction capacity in a reactive distillation column (larger holdup, more reactive trays,

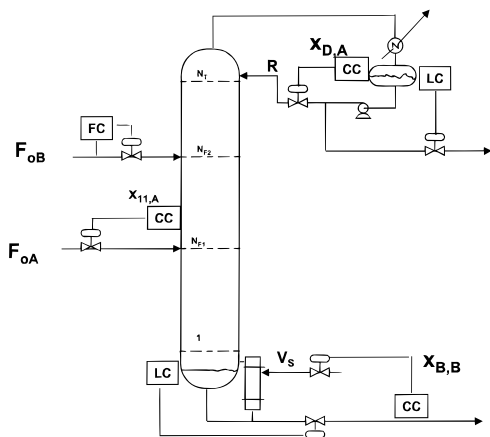


Figure 6. Control structure CS2; control impurities.

or more catalyst) makes the control of the process easier. This is probably the single most important concept that this paper tries to convey. This improvement in controllability with additional reaction capability probably has both steady-state and dynamic components and will be the subject of future work.

3.2. Control Structure CS2. Figure 6 gives a control structure in which, instead of controlling the purities of the two products (the concentration of product components C in the distillate and D in the bottoms), one impurity in each product stream is controlled. At first glance this may appear to be no different than the previous case. In conventional distillation of a binary mixture, that would be true. However, in reactive distillation there are four components and the impurities in the product streams can be either of the reactants. The largest impurity in the distillate is component A because it is the next lightest compared to product C. However, as the composition profiles in Figure 2A show, there are large concentrations of component B up in the rectifying section, so both A or B can find their way overhead. This can occur when there is not enough reaction occurring to consume the reactants. The reverse situation occurs in the bottom, with B being the principle impurity but A capable of dropping out in the bottoms.

The difference in performance can be seen by comparing Figure 4 (purity control) with Figure 7A (impurity control). The disturbance of a 20% increase in the F_{oB} fresh feed is handled in Figure 4 (using the P controller) but is not handled by the impurity control structure in Figure 7A. Both reflux flow and vapor boilup keep increasing and reach saturation after about 4 h.

This configuration also cannot handle changes in setpoints, as illustrated in Figure 7B. Making a small change in the impurity of B in the bottoms from 5% to 4% can be handled, but making only a slightly larger change in the impurity of A in the distillate from 5% to 3% produces instability and saturation of reflux and vapor boilup.

3.3. Control Structure CS3. Instead of controlling both product purities, it may be possible in some systems to only control one product and overpurify the other product. Single-end control is simpler and easier to tune and gives faster response because of the reduced interaction among the control loops. Figure 8 shows a control structure using this strategy. The reflux-drum level is controlled by manipulating the reflux, and a constant reflux ratio (equal to the steady-state value) is maintained by adjusting the distillate flow rate.

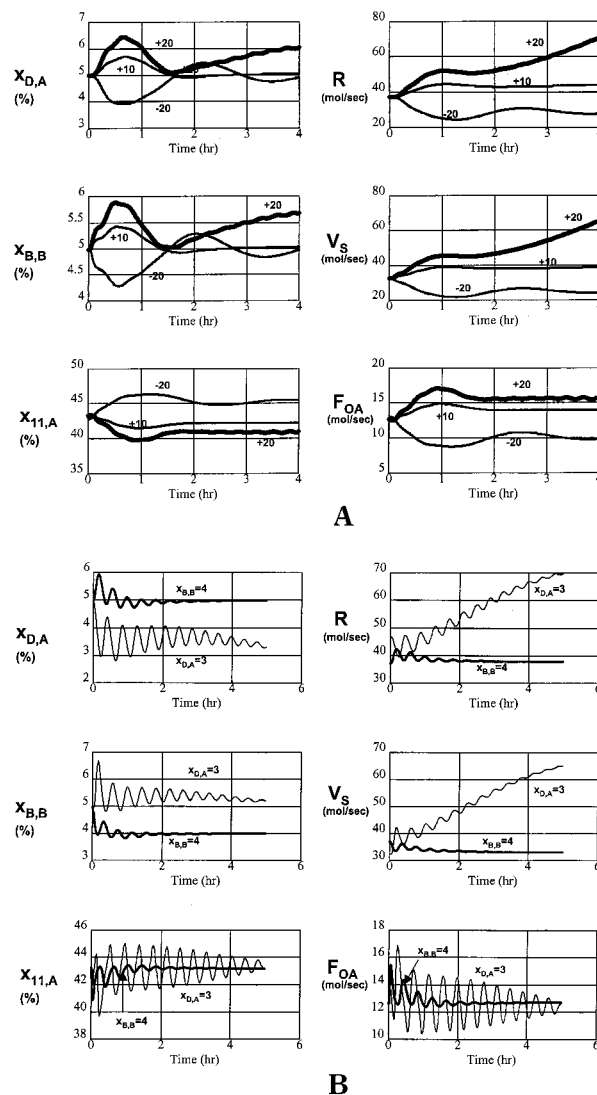


Figure 7. (A) CS2; -20% , $+10\%$, $+20\%$ F_{oB} . (B) CS2; $x_{D,A}$ changed to 3% ; $x_{B,B}$ changed to 4% .

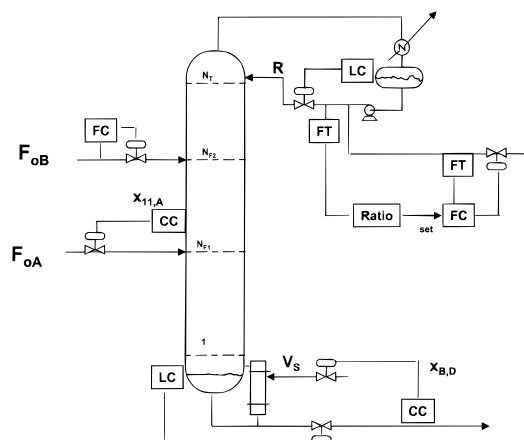
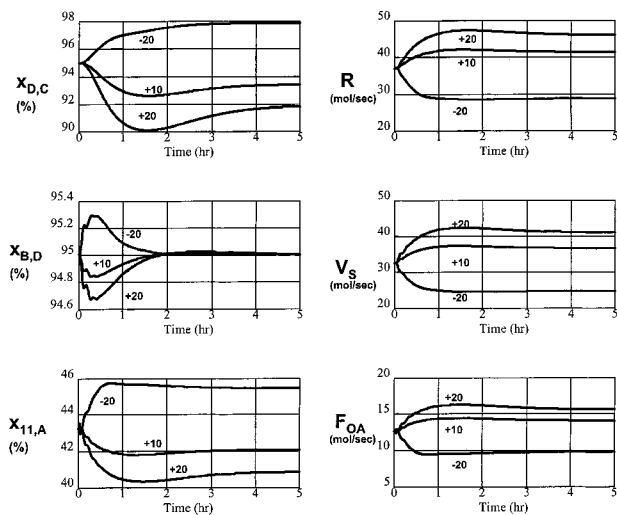


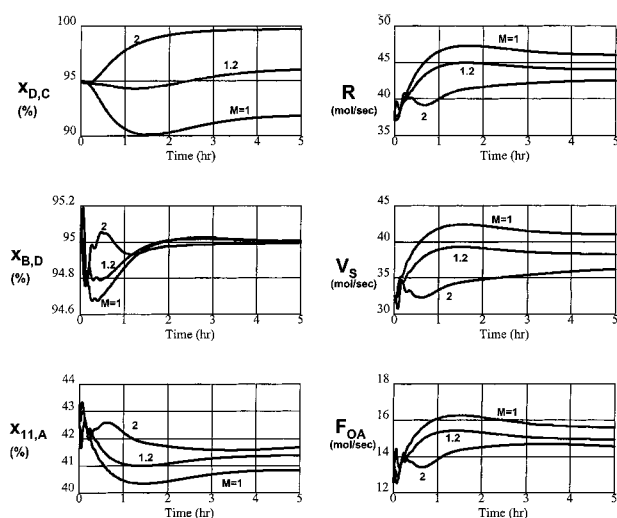
Figure 8. Control structure CS3; single-end control.

Bottoms product purity is controlled by manipulating the vapor boilup. Distillate purity is not controlled.

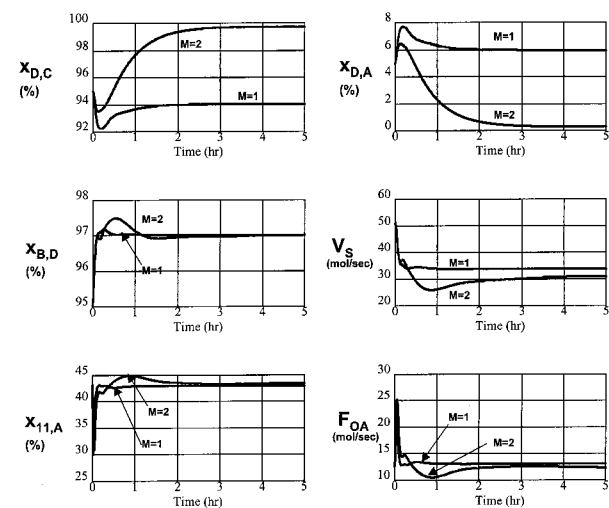
Figure 9A shows that large changes in the throughput can be easily handled, and the response of the system is faster. However, at the higher production rates, the distillate product falls below its specified purity. Figure 9B shows that the distillate purity can be kept above the 95% specification if the tray holdups are increased



A



B



C

Figure 9. (A) CS3; -20% , $+10\%$, $+20\%$ changes in F_{OB} . (B) CS3; $+20\%$ change in F_{OB} ; $M = 1, 1.2,$ and 2 . (C) CS3; $x_{B,D} = 0.97$ ($M = 1$ and 2).

from the base case 1 kmole to 1.2 kmoles. Even higher tray holdups give higher purity distillate for the same bottoms purity and the same reflux ratio.

Figure 9C gives responses to an increase in the

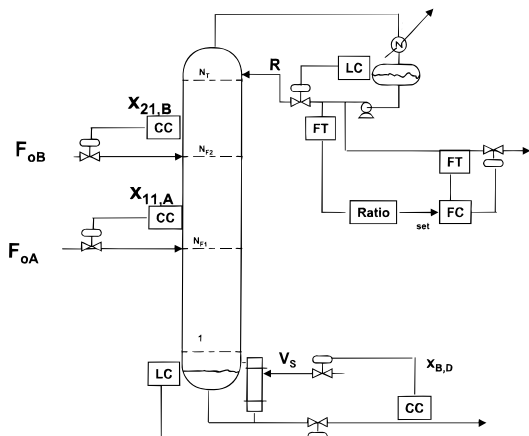


Figure 10. Control structure CS4; manipulate both fresh feeds.

setpoint of the bottoms purity controller from 95% to 97% for two different tray holdups. The higher tray holdups result in higher distillate purity.

Thus, this example again demonstrates that overdesigning the reactive section makes dynamic control easier. Only one end of the column needs to be controlled. Load response is faster. The uncontrolled product is always above specification.

3.4. Control Structure CS4. Figure 10 gives a control scheme in which two compositions in the column are controlled, one at each end of the reactive zone: the composition of A at the bottom of the reactive zone and the composition of B at the top of the reactive zone. This structure was explored because it is similar to what might be done in a conventional process in which the reactor effluent is fed to a separation section. The reactant components would be separated from the product components and recycled back to the reactor. With the volatilities used in this paper, the flowsheet of the conventional process would consist of a reactor and two distillation columns in series. Product C would be removed from the top of the first column and product D from the bottom of the second column. The overhead of the second column would be a mixture of components A and B, and it would be recycled back to the reactor. The two fresh feed streams could be brought in on some type of composition control, perhaps using one composition controller and the reflux-drum level in the second column. The control scheme shown in Figure 10 is conceptually similar. It also has some similarities with the scheme proposed by Roat et al.¹¹ in which the two fresh feed streams control two tray temperatures.

Figures 11 and 12 demonstrate that this structure works well. The production rate can be changed by adjusting the setpoints of either (or both) of the reaction-zone composition controllers (Figure 11). Product purity changes are also effectively handled (Figure 12).

Of course, this structure has two disadvantages: (1) two composition analyzers are required and (2) there is no direct production-rate handle.

3.5. Control Structure CS5. Instead of using bottoms composition control, it is possible in the system studied in this paper to use a tray temperature in the stripping section. Tray 5 is selected because it is where there is a significant break in the temperature profile. Figure 13 shows the control scheme. Single-end control with constant reflux ratio control is used.

Figure 14A shows the response of the system for a 20% increase in the F_{OB} fresh feed flow rate. Two curves

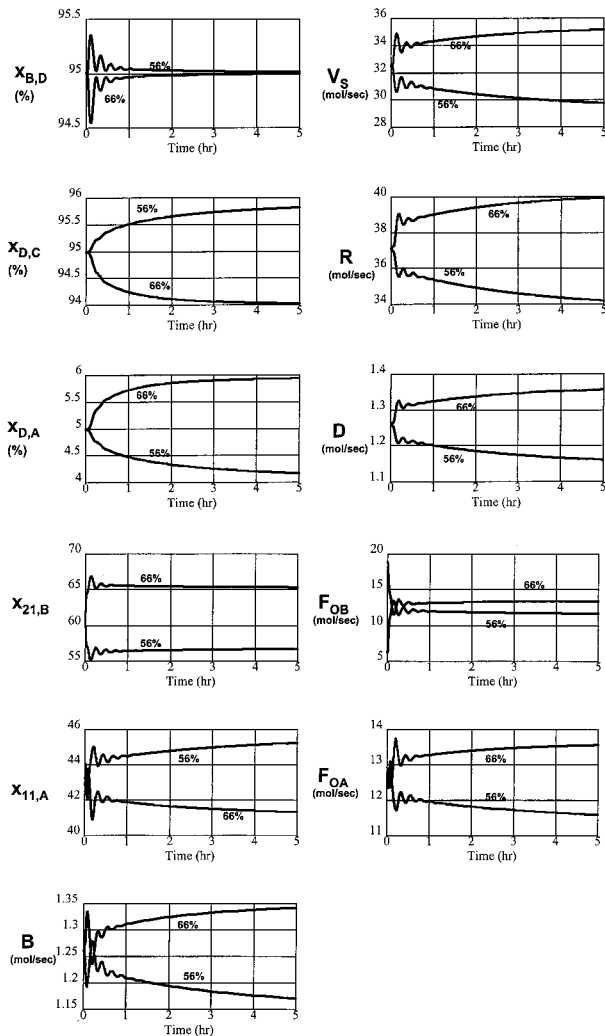


Figure 11. CS4; $\pm 5\%$ changes in the setpoint of $x_{2,2,B}$.

are shown corresponding to two tray holdups. With the base-case holdup of 1 kmol/tray, the temperature controller does a good job in maintaining the purity of the bottoms, but the overhead purity drops. When tray holdup is increased to 2 kmol, distillate purity is above specification. Notice that the F_{OA} fresh feed flow rate increases more for the $M = 1$ case than for the $M = 2$ case. This is because there is more A being lost out the top when the distillate purity is low.

Figure 14B demonstrates that temperature setpoint changes are easily handled. Product purities change in opposite directions, as we would expect.

3.6. Control Structure CS6. The final control scheme explored is shown in Figure 15. The distillate product purity is controlled by manipulating the F_{OB} fresh feed flow rate. This scheme feeds as much to the column as it can handle with the specified reflux ratio and tray 11 composition of component A. There is no direct production-rate handle.

Figure 16A shows that the scheme maintains distillate product purity in the face of changes in the setpoint of the bottoms purity controller. Increasing the bottoms purity leads to a reduction in the throughput (both the F_{OA} and F_{OB} fresh feed flow rates decrease). Figure 16B shows that an increase in tray holdup results in higher throughputs despite the increase in bottoms purity. Figure 16C illustrates that this structure alters production rates to match the reaction and separation capacity

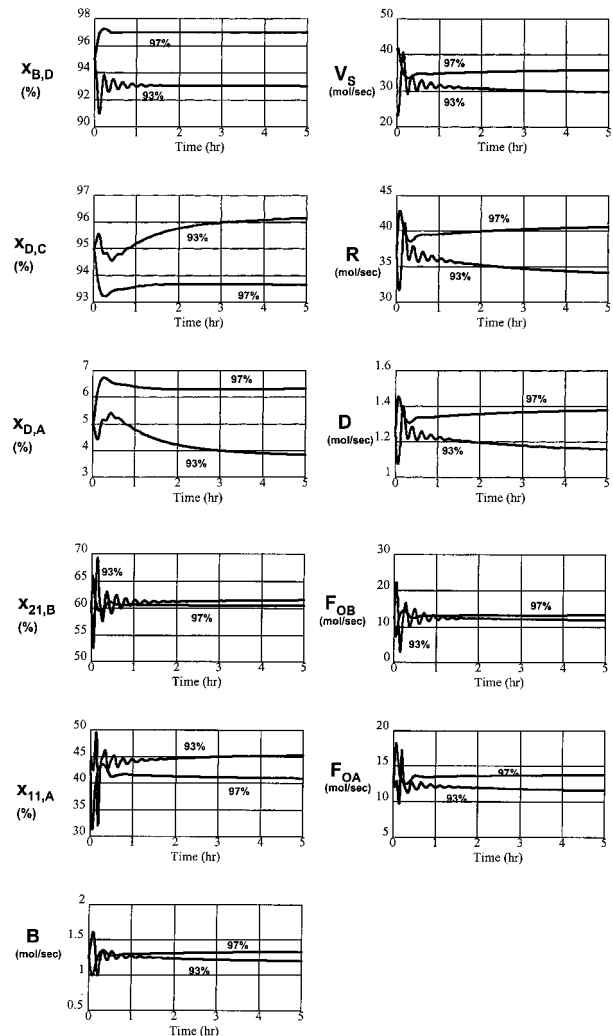


Figure 12. CS4; $x_{B,D}$ changed to 0.97 and 0.93.

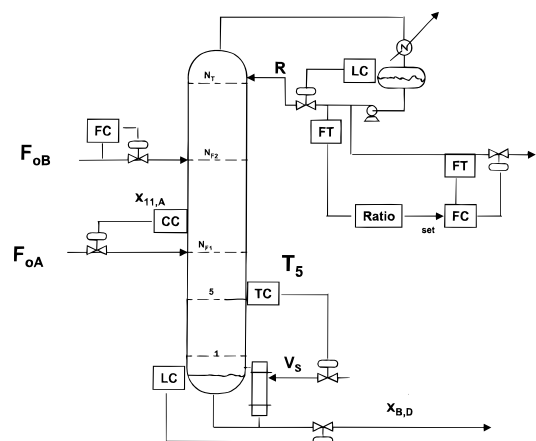


Figure 13. Control structure CS5; single-end temperature control.

of the column. Increasing the pressure raises temperatures and reaction rates, which produces an increase in the throughput. Of course, if pressure were increased too much, the decrease in the reaction equilibrium constant would adversely affect the reaction zone, and production rate would decrease. Reducing the reflux ratio changes the separating capacity of the column and results in lower throughput. If catalyst poisoning occurs, feed compositions change or other disturbances occur,

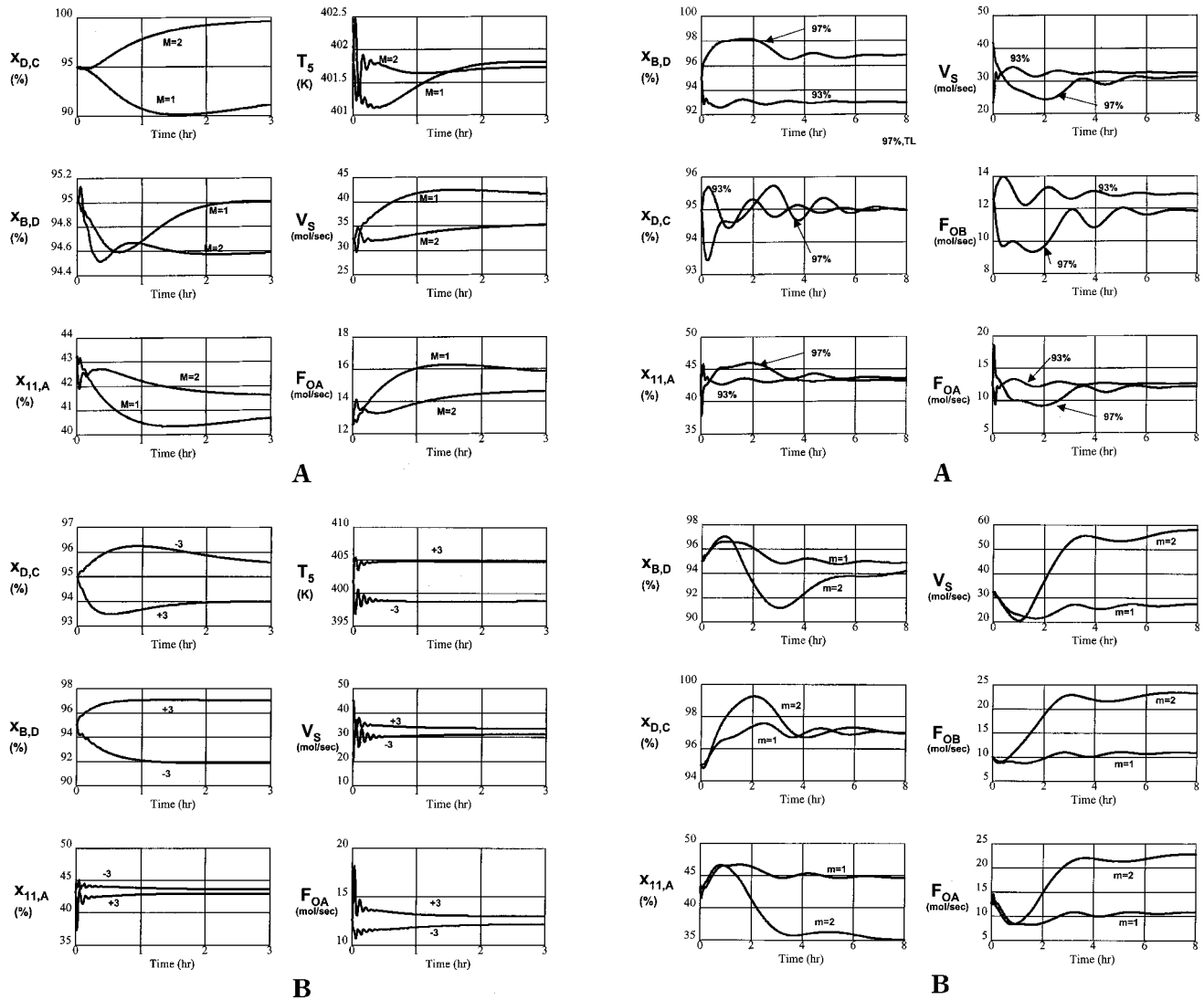


Figure 14. (A) CS5; +20% change in F_{OB} ($M = 1$ and 2). (B) CS5; change in tray 5 temperature.

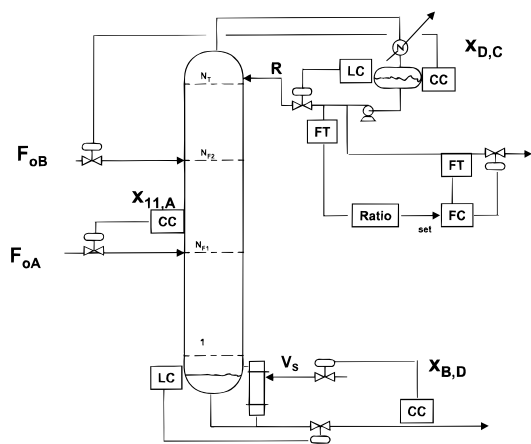


Figure 15. Control structure CS6; manipulate F_{OB} to control $x_{D,C}$.

this scheme finds the feed rates that the column can handle with the specified reflux ratio.

The dynamics of the scheme are slower than the others (note the time scale) because of the lags in the distillate composition to the fresh feed loop.

3.7. Constraint Control. Override control systems have not been shown in any of the schemes, but they

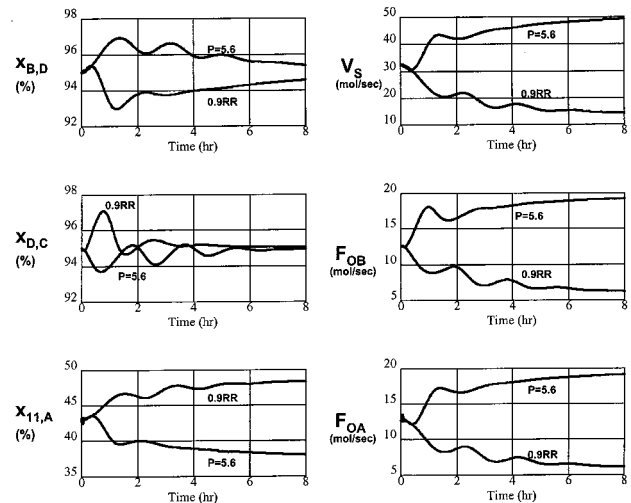


Figure 16. (A) CS6; $x_{B,D}$ changed to 0.97 and 0.93. (B) CS6; $x_{D,C}$ changed to 0.97 ($M = 1$ and 2). (C) CS6; reflux ratio reduced 10%; pressure increased 0.5 bar.

should be incorporated to handle constraints. For example, if the vapor boilup valve saturates wide open, an override strategy should be in place that will cut back on the column feed and still maintain product purity.

4. Conclusion and Future Work

In this paper we have explored a variety of control structures for an ideal two-product reactive distillation column. The impact of the design of the column on the ease of dynamic control has been demonstrated. Single-end control can be used if the reaction zone of the column is provided with plenty of capacity (holdup or catalyst). A wide variety of quite large disturbances can be handled.

Unless an excess of one of the reactants is incorporated in the process design, some detection of the inventory of one of the reactants in the column is required so that a feedback trim can balance the reaction stoichiometry.

Further studies are underway to develop effective control structures for a variety of specific chemical reactive distillation systems. There are a large number of cases because of the variety of chemical reactions, number of products produced, number of fresh feed streams, presence of inert components in the feed, etc. The ethylene glycol system has two fresh feed streams, two consecutive reactions, and one product leaving from the bottom of a totally refluxed column. ETBE and MTBE are similar: either one mixed feed or two separate feeds, inert components in one of the feeds that leave in the overhead of the column, and one product that leaves out of the bottom. Methyl acetate is similar to the ideal case considered in this paper: two feeds and two products.

All of this variety in the processes will probably mean that different control structures will be required. However, the fundamentals of plantwide control²⁰ will apply: accounting for component balances, controlling product quality, satisfying constraints, and handling recycles (in this case, internal to the column).

Nomenclature

a_B = preexponential factor for the reverse reaction ($\text{kmol}\cdot\text{s}^{-1}\cdot\text{kmol}^{-1}$)
 a_F = preexponential factor for the forward reaction ($\text{kmol}\cdot\text{s}^{-1}\cdot\text{kmol}^{-1}$)
 A = reactant component
 B = reactant component
 B = bottoms flow rate (kmol/s)
 C = product component
 D = product component
 D = distillate flow rate (kmol/s)
 E_B = activation energy of the reverse reaction (cal/mol)
 E_F = activation energy of the forward reaction (cal/mol)
 F_{OA} = fresh feed flow rate of reactant A (kmol/s)
 F_{OB} = fresh feed flow rate of reactant B (kmol/s)
 k_F = specific reaction rate of the forward reaction ($\text{kmol}\cdot\text{s}^{-1}\cdot\text{kmol}^{-1}$)
 k_B = specific reaction rate of the reverse reaction ($\text{kmol}\cdot\text{s}^{-1}\cdot\text{kmol}^{-1}$)
 L_n = liquid flow rate from tray n (kmol/s)
 M_n = liquid holdup on tray n (kmol)
 N_R = number of rectifying trays
 N_{RX} = number of reactive trays
 N_S = number of stripping trays
 P = total pressure (bar)
 P_j^s = vapor pressure of component j (bar)
 R = reflux flow rate (kmol/s)
 R = perfect gas law constant ($\text{cal}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$)
 \mathcal{R}_C = rate of production of C (kmol of C /s)
 T_n = temperature in tray n (K)
 V_n = vapor flow rate from tray n (kmol/s)

V_S = vapor boilup (kmol/s)

x_{nj} = composition of component j in liquid on tray n (mole fraction)

y_{nj} = composition of component j in vapor on tray n (mole fraction)

α_j = relative volatility of component j

ΔH_v = heat of vaporization (cal/mol)

λ = heat of reaction (cal/mol of C produced)

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