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ANALYSIS OF CONTROL STRUCTURE FOR RECYCLED REACTION/SEPARATION PROCESSES WITH FIRST ORDER REACTION

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Abstract
Behavior of reaction/separation processes with recycle is different from the configuration with no recycle. A major difference is the instability of recycle processes due to the snowball effect in the presence of a disturbance in feed stream. In the balanced control scheme, snowball effect can be prevented by distribution of load through the process, but it can complicate the control system and increase the concentration control loops. In this paper different methods for avoiding the snowball effect are studied through steady state analysis. Control structures used in this paper are based on the balanced control idea. It is shown that for the two proposed control structures, by using only one concentration control loop, the reactor outlet and product concentrations can be controlled if the disturbances occur in the feed stream.

Keywords: *control structure, recycle, disturbance rejection, snow ball effect.*

Introduction

A chemical plant includes independent operating units such as reactors, distillation columns, heat exchangers and so on. There is a distinct difference between the steady state and dynamic behaviors of these units when they are used in an interconnected system, especially when there is a recycle in the plant. Although the recycle reduces the cost, it has some disadvantages from the control point of view. Luyben [1] showed that changes in concentration and feed flow rate may result in the snowball phenomenon for the processes with recycle. Snowball effect implies that a slight change in the inlet feed flow rate causes a significant change in the flow rate of recycle. This effect may act as a positive feedback and cause instability of the whole system. For prevention of snowball effect, balanced control idea is suggested by Wu and Yu [2]. Balanced control means distributing the effect of load on different parts of the process. This improves the ability of control structure in load rejection and disturbances with larger magnitudes can be rejected. On the other hand the balanced control scheme increases the complexity of the control structure and also the number of concentration loops.

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Adding concentration measurements introduce additional lags into the system dynamic and increase the cost. In this paper we will examine structures based on the idea of balanced control, using only one concentration loop, and compare them with the structures suggested in the literature [2,3]. Denn [4] showed that recycle increases the response time of the process. Luyben in several articles studied the snowball effect for reaction/separation processes. In the first paper [5], he investigated the effect of the recycle loop gain on the stability of the system. In the second paper [6], he studied the effects of the reactor and distillation columns' sizes on the controllability of the processes including recycle loop and showed that by increasing the reactor size, the gain of recycle loop decreases and leads to controllability enhancement. In the third paper [7], he suggested various structures for the controlling a process including one reactor, two distillation columns and one recycle loop.

The paper is organized as follows: First, process description and assumptions used in simulation, are presented. Second, balanced control will be explained. Third, control structures will be proposed and finally they will be compared through simulation.

Process Description

Process includes one reactor and one distillation column [8], according to the Figure 1. The fresh feed of component A enters the reactor and an exothermic irreversible first order reaction (A→B) takes place in the liquid phase. Effluent of the reactor that includes a mixture of (A) and (B), enters the distillation column for separation. Since the volatility of component (A) is more than component (B), it is separated as overhead product and recycled to the reactor. In the Table 1, steady state conditions and parameters of the process are presented.

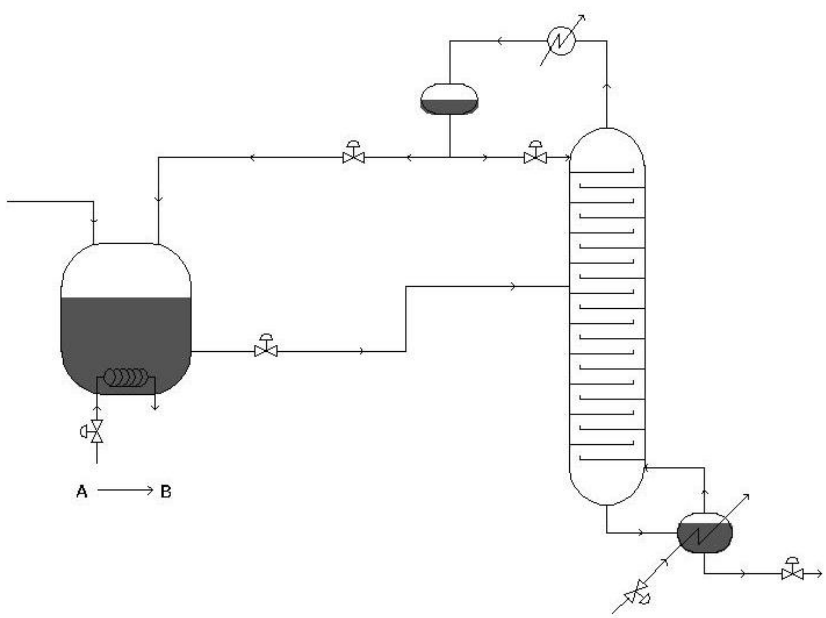

Figure 1- Process including one reactor and one distillation column.

Table 1- Steady state values used for simulation

Feed flow rate to reactor	$F_0 = 3.351 \quad (\text{kmol/min})$
Effluent of reactor	$F = 7 \quad (\text{kmol/min})$
Recycle flow rate	$D = 3.649 \quad (\text{kmol/min})$
Reactor holdup	$V_R = 250 \quad (kmol)$
Reflux drum holdup	$V_{ref} = 20 \quad (\text{kmol})$
Reboiler holdup	$V_{reb} = 30 \quad (\text{kmol})$
Reaction constant	$k_0 = 2.48*10^8 \quad (\text{min}^{-1})$
Activation energy	$E = 70000 \quad (\text{kJ/kmol})$
Heat of reaction	$\Delta H_r = 70000 \quad (\text{kJ/kmol})$
Feed concentration	$z_0 = .9$
Reactor effluent concentration	$z = .5$
Top concentration of distillation column	$X_D = .95$
Bottom Concentration of distillation column	$X_B = .01$

Controlling structures are independent of the physical properties, and these structures are applicable to all materials. It should be mentioned that for the performed simulation, Simulink software, in MATLAB package, has been used.

Assumptions used in simulation are as follows:

- Vapor phase hold-up is neglected
- Changing of liquid phase heat capacity with temperature is neglected
- Condenser pressure is constant at one atmosphere
- Condenser hold-up is constant
- Condenser operates under total condensation
- Lag due to liquid flow transfer from the reactor to the distillation column is neglected
- Measurement lags are neglected
- Control valves dynamics are neglected

Data used for simulation of distillation column are as follows:

- Number of column trays: $N_T = 20$
- Active surface of trays: $A_{tray} = 3\,m^2$
- Total tray holes surface: $A_{hole} = .36\,m^2$
- Tray weir length: $Length_{weir} = 1.1\,m$
- Height of tray weir: $height_{weir} = .1\,m$
- Inlet nozzle diameter of condenser: $D_{pipe} = .18\,m$

Controllers tuning

Controllers used in this work are the proportional-integral type (PI). For single loop tuning (except flow controllers), the Cohen-Coon method is used and for detuning, due to interaction and recycle effects on control loops, the controller parameters are changed by trial and error to obtain the decay ratio of 1/4. Flow controllers are tuned by the quarter decay ratio technique.

Balanced control idea

Steady state relations of the process play an important role in the analysis of the processes with recycle loop.

Steady state mass balance for the reactor yields [2]:

$$F_{in} + D = F \tag{1}$$

$$F_{in} \cdot z_{in} + D \cdot X_D = F \cdot z + V_R \cdot k \cdot z \tag{2}$$

Distillation column steady state mass balance results in:

$$\mathrm{F} = \mathrm{B} + \mathrm{D} \tag{3}$$

$$F \cdot z = B \cdot X_B + D \cdot X_D \tag{4}$$

By writing the total mass balance, we have:

$$F_{in} = B \tag{5}$$

From equations 2, 4 and 5, we have:

$$F_{in}\left(z_{in} - X_B\right) = V_R \cdot k \cdot z \tag{6}$$

From equations 3,4 and 5, we get:

$$\frac{F}{F_{in}} = \frac{X_D - X_B}{X_D - z} \tag{7}$$

Equations 6 and 7 show functionality of process variables with feed flow rate and concentration under steady state condition. Combining equations 6 and 7 yields:

$$\frac{F}{F_{in}} = \frac{V_R \cdot k\left(X_D - X_B\right)}{V_R \cdot k \cdot X_D - F_{in}\left(z_{in} - X_B\right)} \tag{8}$$

Equation 8 shows the relation between the reactor hold-up (level) and the reactor effluent flow rate that can be used for disturbance rejection.

Figure 2 shows the reactor hold-up, V_R, versus the reactor effluent flow rate under steady state condition and perfect control of overhead and bottom product compositions.

Each curve in Figure 2 shows collection of steady state points that have the same ability for rejection of disturbances caused by feed flow rate changes. Point D shows the initial steady state. Points A1, A2 and A3, are related to the structures that disturbances due to feed flow rate changes are rejected only by changing the reactor hold-up (level control) while reactor effluent flow rate stays constant. In other words, the disturbance is rejected in the reactor and distillation column has no role in disturbance rejection.

Points C1, C2 and C3, are related to the structures that disturbances are rejected only by changing the reactor effluent flow rate while reactor hold-up, remains constant. In other words, the disturbance is rejected in the distillation column and the reactor (control level) has no role in disturbance rejection. However, there are infinite steady state points with the ability of disturbance rejection by dividing its effect on the performances of reactor and distillation column.

Considering the physical constraints (reactor volume and increasing of inlet flow to the distillation column), a steady state point can be selected and an appropriate control structure can be designed based on the steady state analysis of disturbance [2,9].

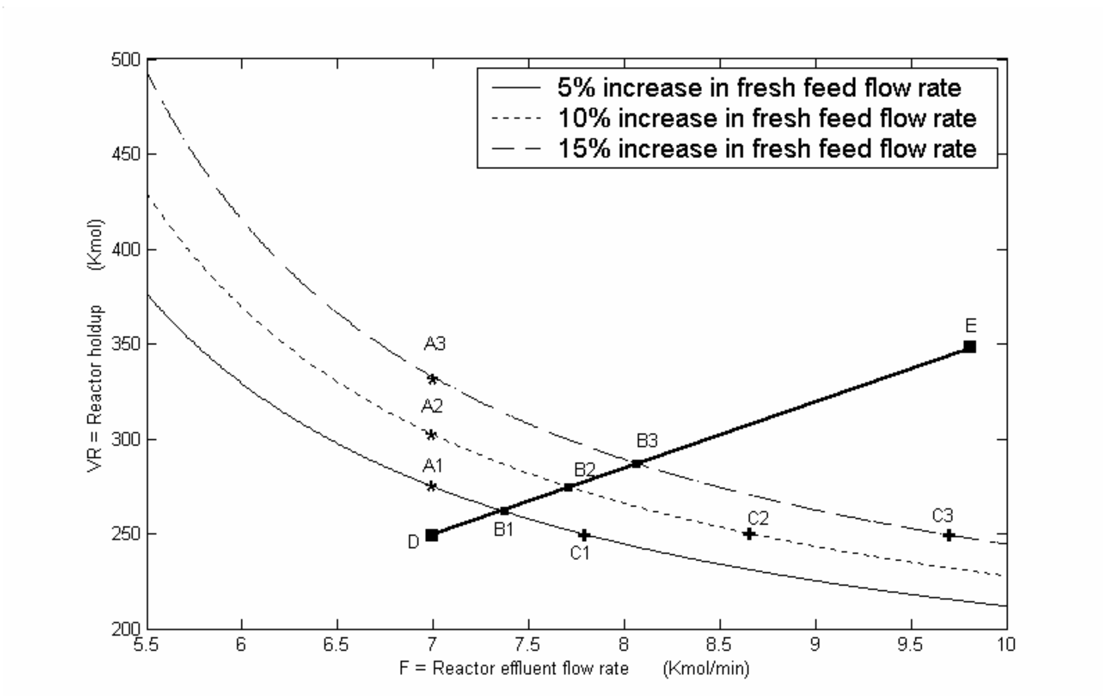

Figure 2- Reactor holdup versus reactor effluent flow rate.

Proposed structures in this paper are designed for keeping the steady state condition on the DE line (Fig. 2) after disturbance rejection. It is clear that the new steady state point may be placed on various points of the DE line.

Steady state analysis of disturbance

If equations 6, 7 and 1, are written for the initial (with subscript 0) and final (with subscript ∞) steady state and assuming perfect control of top and bottom product concentrations, it can be shown that [2]:

$$\left(\frac{V_{R,\infty}}{V_{R,0}}\right) = r \text{ Or } V_R^* = r - 1 \qquad (9)$$

$$\left(\frac{F_\infty}{F_0}\right) = r \text{ Or } F^* = r - 1 \qquad (10)$$

$$\left(\frac{D_\infty}{D_0}\right) = r \text{ Or } D^* = r - 1 \qquad (11)$$

where $r = \frac{F_{in,\infty}}{F_{in,0}}, F_{in}^* = r - 1$. Variables with superscript * are defined as $y^* = \frac{y_\infty - y_0}{y_0}$. It should be noted that in developing the above equations, it is assumed that z_{in} is constant.

In a similar way for changing in the feed composition, while the feed flow rate remains constant, the following equations can be derived:

$$\left(\frac{V_{R,\infty}}{V_{R,0}}\right) = \frac{z_{in,\infty} - X_B}{\bar{z}_{in,0} - X_B} \text{ Or } V_R^* = \frac{z_{in,\infty} - z_{in,0}}{z_{in,0} - X_B} \quad (12)$$

$$\left(\frac{F_\infty}{F_0}\right) = 1 \text{ Or } F^* = 0 \quad (13)$$

$$\left(\frac{D_\infty}{D_0}\right) = 1 \text{ Or } D^* = 0 \quad (14)$$

Equations 9 to 11 can be presented in a sensitivity analysis frame [3]:

$$\left(\frac{\partial V_R{}^*}{\partial F_{in}^*}\right)_{X_D, X_B, z} = 1 \quad (15)$$

$$\left(\frac{\partial F^*}{\partial F_{in}^*}\right)_{X_D, X_B, z} = 1 \quad (16)$$

$$\left(\frac{\partial D^*}{\partial F_{in}^*}\right)_{X_D, X_B, z} = 1 \quad (17)$$

Equations 15 to 17 show that the steady state gain of the variables V_R^*, F^* and D^* respect to the disturbance F_{in}^* is equal to one.

In the same way, the steady state gain can be calculated for other variables. For example, from equation 5, the steady state gain of variable B can be obtained as follows:

$$\left(\frac{\partial B^*}{\partial F_{in}^*}\right)_{X_D, X_B, z} = 1 \quad (18)$$

From equation 16 we have [2]:

$$\left(\frac{\partial R^*}{\partial F_{in}^*}\right)_{X_D, X_B, z} \approx 1 \quad (19)$$

$$\left(\frac{\partial V^*}{\partial F_{in}^*}\right)_{X_D, X_B, z} \approx 1 \quad (20)$$

where R^* and V^* represent the normalized reflux flow and the reboiler steam flow rate, respectively.

In the same way for disturbance in z_{in}, we have:

$$\left(\frac{\partial V_R^*}{\partial z_{in}}\right)_{X_D, X_B, z} = \frac{1}{z_{in,0} - X_B} \quad (21)$$

The changes in z_{in} has no effect on R^* and B^*.

If equations 15 to 21 are written in the matrix form, the following equation will be achieved which includes the steady state disturbance sensitivity matrix [3]:

$$\begin{bmatrix} V_R^* \\ F^* \\ D^* \\ B^* \\ R^* \\ V^* \end{bmatrix} = \begin{bmatrix} 1 & \frac{1}{z_{in} - X_B} \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} F_{in}^* \\ z_{in} \end{bmatrix} \quad (22)$$

Control Structures

As it was mentioned before, using the concentration measurement is undesirable due to its lag and cost, therefore the control structures with minimum concentration control loops are preferred. One simple solution for this goal is using the ratio controller. From equation 10 we get:

$$\left(\frac{\partial \left(F^* / F_{in}^* \right)}{\partial F_{in}^*} \right)_{X_D, X_B, z} = 0 \quad (23)$$

In the same way, we have:

$$\left(\frac{\partial \left(F^* / F_{in}^* \right)}{\partial z_{in}} \right)_{X_D, X_B, z} = 0 \quad (24)$$

Equations 23 and 24 indicate that the feed flow rate and concentration changes have no effect on the ratio of the reactor effluent to feed flow rate.

Considering the above fact, the disturbance sensitivity matrix can be written in the following form:

$$\begin{bmatrix} V_R^* \\ \left(F^* / F_{in}^* \right) \\ D^* \\ B^* \\ R^* \\ V^* \end{bmatrix} = \begin{bmatrix} 1 & \frac{1}{z_{in} - X_B} \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} F_{in}^* \\ z_{in} \end{bmatrix} \quad (25)$$

For controlling X_D, X_B and z it is necessary to use three concentration loops. From equation 25 it is clear that changes in feed flow rate and composition have no effect on the F^* / F_{in}^* ratio. Also from equation 7 it is clear that X_D, X_B and z can be controlled by using only two concentration loops. Therefore two variables from X_D, X_B and z must be controlled. Control of product concentration is important and therefore X_B is selected as the first variable. Now we must select the second variable from z and X_D , and therefore we have two alternatives.

Balratio(F/Fin)- XB-z Structure

For control of reactor concentration we can use flow rates F or D. In this structure, ratio F^* / F_{in}^* is constant and therefore we can only use the flow rate of D for control of reactor concentration. For control of X_B we can use the steam flow rate. Ratio control loop is used for the reactor to avoid the third concentration control loop.

Balratio(F/Fin)- XD-XB Structure

This structure has been proposed by wu & yu [2]. The disturbance sensitivity matrices of this structure and the previous one are the same.

Balratio(F/D)- XB-XD Structure

In this structure by using steady state disturbance analysis and use of a ratio controller, one of the concentration control loops has been eliminated. Difference between this structure and the two previous ratio control structures, is replacing (F^* / F_{in}^*) by (F^* / D^*).

In this case disturbance sensitivity matrix has the following form:

$$\begin{bmatrix} V_R^* \\ \left(F^*/D^*\right) \\ D^* \\ B^* \\ R^* \\ V^* \end{bmatrix} = \begin{bmatrix} 1 & \dfrac{1}{z_{in} - X_B} \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} F_{in}^* \\ z_{in} \end{bmatrix} \qquad (26)$$

In this structure concentrations X_D and X_B are controlled and the reactor holdup is used for controlling the ratio F^* / D^*.

Figures 3 and 4 show the variations of reactor effluent recycle flow, reactor outlet concentration and reactor holdup for the three aforementioned structures due to ±10% changes in the feed flow rate. In another work, Luyben [8] proposed two balanced control structures with only one concentration loop, called B_C1 and B1_a. In the former one the ratios of V^* / B^* and R^* / D^* are controlled while in the latter one, the ratios of F^* / F_{in}^* and V^* / B^* are being controlled.

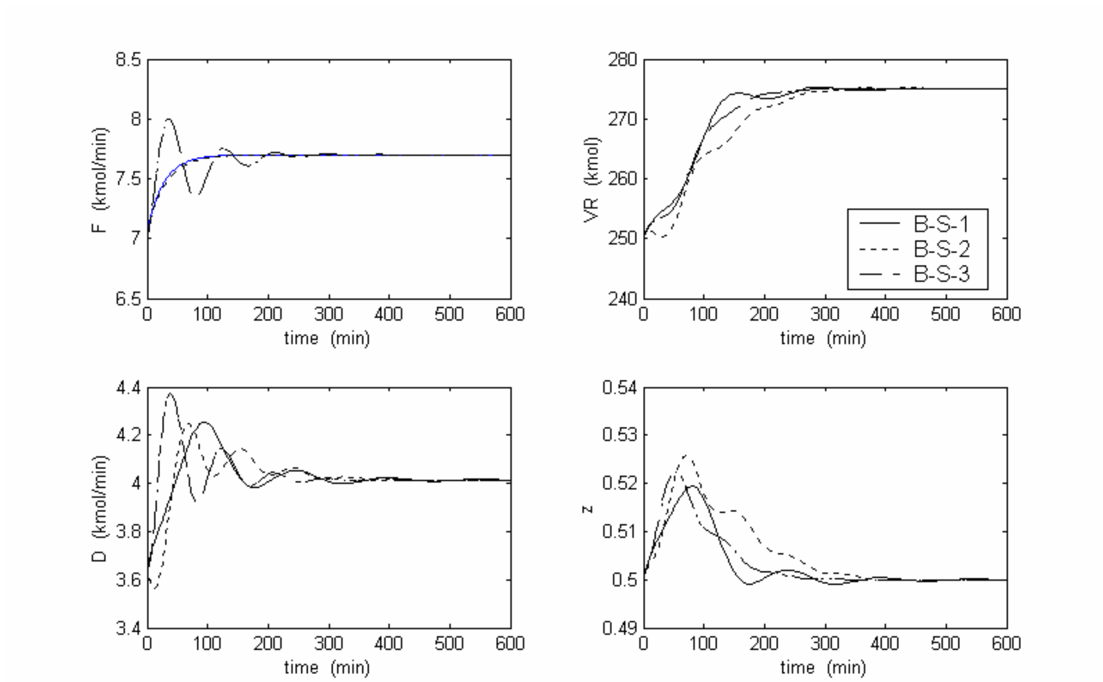

Figure 3- Variations of system states versus time for the three control structures with two concentration loops due to 10% increase in feed flow rate.

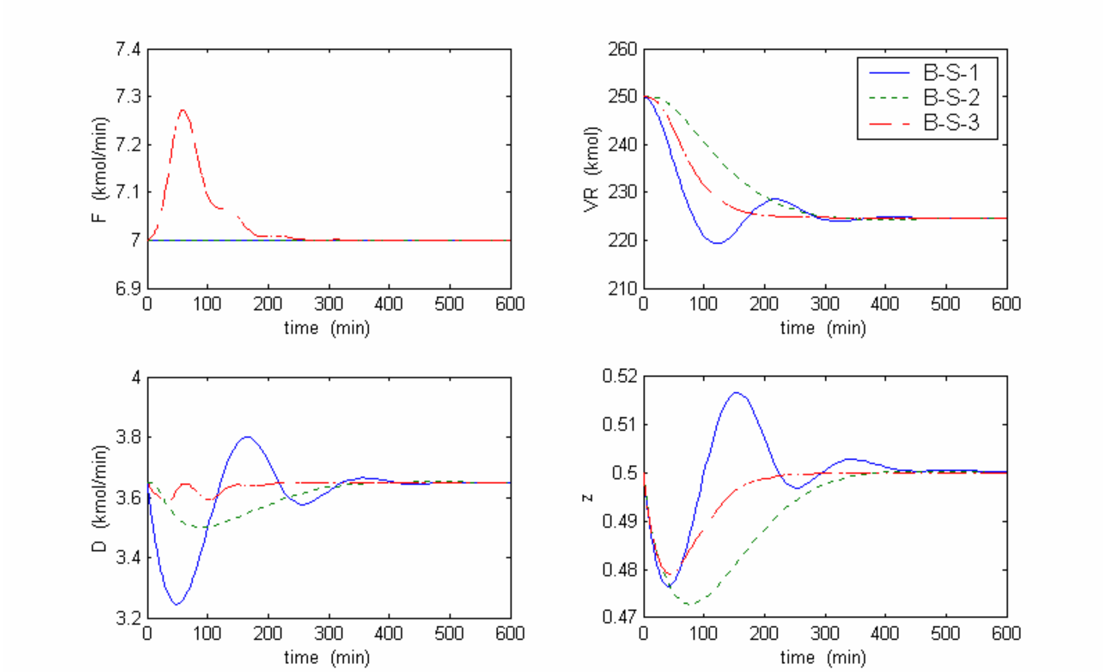

Figure 4- Variations of system states versus time for the three control structures with two concentration loops due to 10% decrease in feed flow rate.

First proposed control structure

Similar to structures B_C1 and B1_a, in the proposed control structure only one concentration control loop has been used. By some manipulation the sensitivity disturbance matrix can be written in the following form:

$$\begin{bmatrix} V_R^* \\ \left(F^*/F_{in}^*\right) \\ (D^*/R^*) \\ B^* \\ R^* \\ V^* \end{bmatrix} = \begin{bmatrix} 1 & \dfrac{1}{z_{in} - X_B} \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} F_{in}^* \\ z_{in} \end{bmatrix} \qquad (27)$$

Equation 27 indicates that X_D , X_B and z can be controlled by using only one concentration loop. The schematic diagram of the proposed control structure is depicted in Figure 5. As can be seen two ratio control loops (F^*/F_{in}^* and D^*/R^*) have been used and the bottom product composition is controlled by manipulating the steam flow rate to the reboiler.

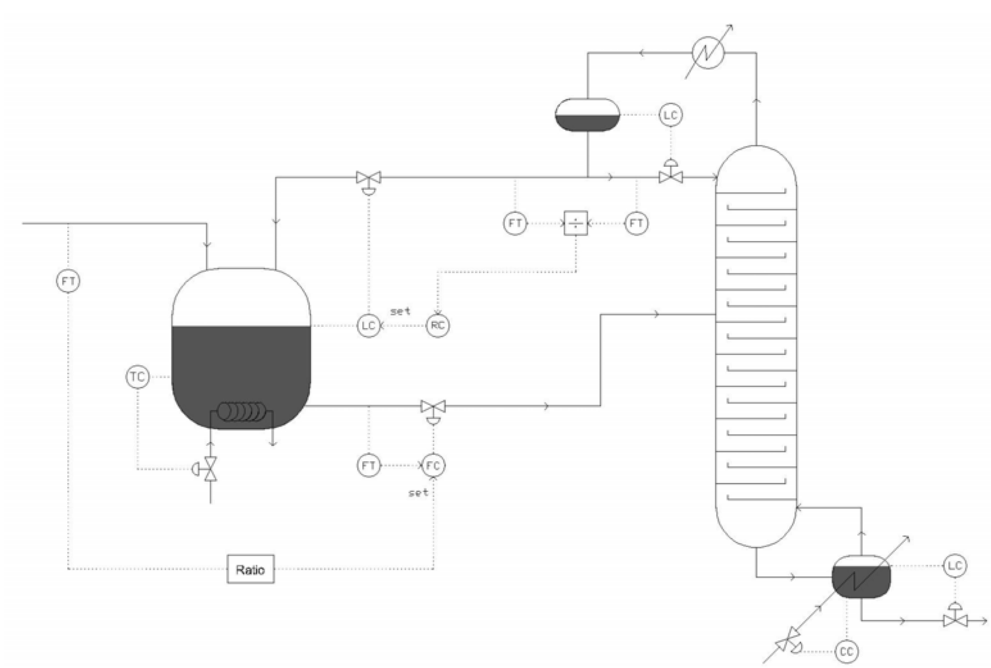

Figure 5- First proposed control structure.

Second proposed control structure

This structure is similar to the previous one, except the ratio control loops are different. Again by some manipulation the sensitivity disturbance matrix can be written in the following form:

$$\begin{bmatrix} V_R^* \\ \left(F^*/D^*\right) \\ (R^*/F^*) \\ D^* \\ B^* \\ V^* \end{bmatrix} = \begin{bmatrix} 1 & \dfrac{1}{z_{in} - X_B} \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} F_{in}^* \\ z_{in} \end{bmatrix} \qquad (28)$$

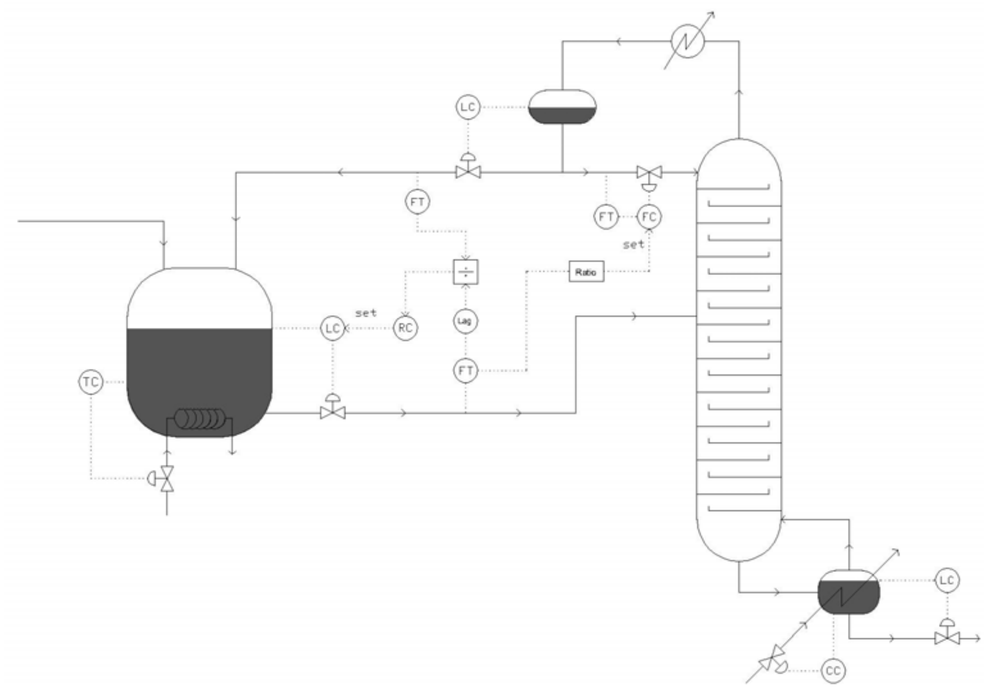

Figure 6- Second proposed control structure.

Equation 28 indicates that X_D , X_B and z can be controlled by using only one concentration loop. The schematic diagram of the proposed control structure is depicted in Figure 6. In this structure the two ratio control loops (F^* / D^* and R^* / F^*) have been used.

Figures 7 and 8 show the variations of reactor holdup, reactor outlet concentration and X_D, X_B for the three structures B-1a, first and second proposed structures due to ±10% changes in feed flow rate.

As can be seen, the performances of the proposed structures are superior. This is due to the faster dynamic of bottom product concentration control loop. In the proposed structures the steam flow rate to the reboiler, which has fast and effective influence on the bottom product composition, has been used for controlling X_B.

Conclusions

In this paper, control of reaction/separation/recycle processes with first order reaction has been considered. Since the composition measurements have lag and are expensive, structures with minimum concentration loops are desired. The main disturbances are feed flow rate and composition and the objective is controlling the reactor outlet concentration, overhead and bottom product compositions. Two control structures based on the sensitivity analysis have been proposed which use only one composition loop. The performances of these structures are compared with one control scheme proposed in the literature. Simulation results indicate that the proposed control structures have faster dynamic responses. This has been achieved due to fast and effective influence of steam flow rate on the bottom product composition.

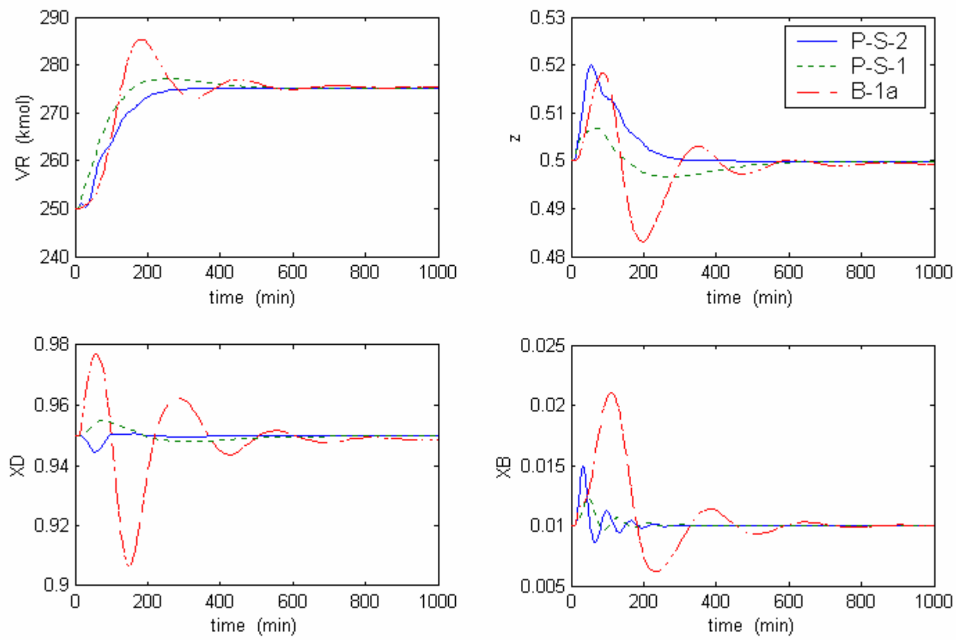

Figure 7- Variations of system states versus time for the structures B_1a, first and second proposed structures due to 10% increases in feed flow rate.

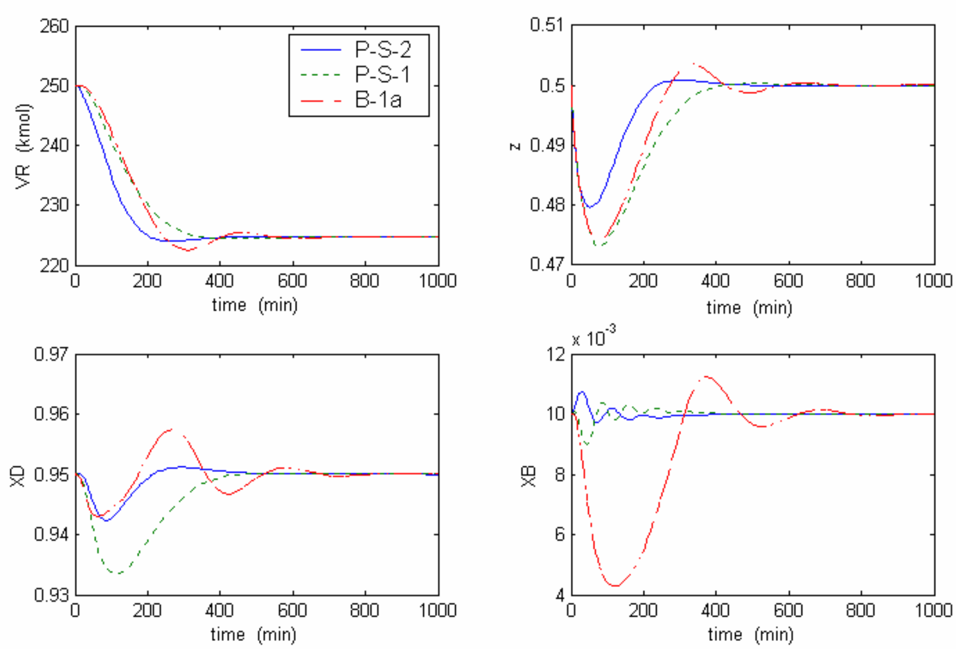

Figure 8- Variations of system states versus time for the structures B_1a, first and second proposed structures due to 10% decreases in feed flow rate.

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