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Reactor/separator processes with recycles-2. Design for composition control

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Abstract

This paper considers the plantwide control structure design for improved disturbance rejection. The balanced control scheme of 'Comput. Chem. Eng. 20 (1996) 1291' has the advantage of alleviating the snowball effect for plants with recycles by changing condition in several units in the process so as to distribute the work evenly among process units as production rate changes. However, the balanced scheme may lead to rather complex control configurations, especially for composition control. Based on steady-state disturbance sensitivity analyses, we are able to simplify the control structure by eliminating some of the compositions loops and still maintain a balanced partial composition control structure. More importantly, this is achieved with minimal process information, i.e., material balances and characteristics of the balanced scheme. For a simple recycle plant, results show that only one composition loop is sufficient to keep all three compositions near set points. A number of single composition control alternatives are explored. Two attractive alternatives are: (1) letting the reactor level uncontrolled or (2) using a proportional only reactor level controller. Nonlinear simulations show that effective composition control can be obtained with rather simple control structures.

Keywords: Plantwide control; Recycle structure; Material recycle; Disturbance rejection

1. Introduction

Dynamics and control of processes with recycles have received little attention until recently. Earlier work on recycle processes focused on the dynamics of reactor/separator systems (Denn & Lavie, 1982; Gilliland, Gould, & Boyle, 1964; Verykios & Luyben, 1978). Luyben and coworkers (Luyben, 1993a,b,c, 1994; Luyben & Luyben, 1995; Tyreus & Luyben, 1993) investigated the effects of recycle loops on process dynamics. The interaction between design and control was also studied for several process systems with different levels of complexity, and a design procedure for plantwide control system was also proposed (Luyben, Tyreus, & Luyben, 1997, 1999).

One of the objectives of process control is to maintain smooth operation in the face of disturbances, upsets or changes in operating conditions. That means the process should remain operable as the production rate, purity of raw materials or product specification change. Luyben (1994) showed that the recycle system may exhibit the 'snowball effect' as feed conditions change. For example, a small change in the fresh feed flow rate could lead to a significant increase in the flow rates of recycle streams. This effect can be severe for systems with a low one-pass conversion that may be unavoidable for highly exothermic reactions where the recycle streams play the role of heat carrier (Luyben, 1994). Similar to the concept of extensive variable control (Georgakis, 1986), a 'balanced' control scheme was proposed by Wu and Yu (1996) to overcome the snowball effect. A balanced control structure handles disturbances by changing conditions in several units in the process, not just one. For example, changing both reactor holdup and recycle flow rate can result in smaller changes in the individual manipulated variables. Better operability can be achieved using the balanced scheme. However, it is

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Nomenclature

$\mathscr{A}$	Reactant
$\mathscr{B}$	Product
B	bottoms flow rate (lbmol/h)
BR	boilup ratio (V/B)
D	distillate flow rate (lbmol/h)
F	reactor effluent flow rate (lbmol/h)
F_0	fresh feed flow rate (lbmol/h)
FR	feed ratio (F/F_0)
h_R	reactor level (%)
K	specific reaction rate (/h)
K_c	controller gain
K_u	ultimate gain
M_B	bottoms holdup (lbmol)
M_D	Condenser holdup (lbmol)
P_u	ultimate period (h)
$\mathscr{R}$	reaction rate (lbmol/h)
R	reflux flow rate (lbmol/h)
RR	reflux ratio (R/D)
RR	recycle ratio (D/B)
T	reactor temperature
V	vapor boilup rate (lbmol/h)
V_R	reactor holdup (lbmol)
x_B	Distillation bottoms composition (mole fraction)
x_D	Distillation top composition (mole fraction)
Z	reactor composition (mole fraction)
z_0	fresh feed composition (mole fraction)
Greek symbols	
τ_I	reset time
Superscripts	
–	nominal value
Set	set point

vital to achieve this 'balance' using the simplest possible control system.

Systematic methods for plantwide control have been developed by several research groups and they range from heuristic-based methodology and optimization-based approach. Yi and Luyben (1995), Semino and Giuliani (1997), Luyben, Tyreus, & Luyben, (1999), Skogestad (2000), Robinson, Chen, McAvoy, and Schnelle (2001) present heuristic approaches for the design of plantwide control systems and to screen possible control configurations. McAvoy (1999), Wang and McAvoy (2001), Bansal, Perkins, and Pistikpoulos (2002) propose optimization-based approaches for plantwide control system synthesis under different level of complexity (ranging from simultaneous design and control to control emphasizing transient). Larsson and Skogestad (2000) give an updated review on plantwide control up to 2000 and Stephanopoulos and Ng (2000) provide comparative analysis for different approaches.

The purpose of this work is to explore several balanced control structures. This paper is organized as follows. The essence of the balanced scheme is studied and disturbance sensitivity is analyzed in Section 2. In Section 3, control structures with different numbers of composition loops are explored and a control structure design procedure is proposed. Dynamics and control of different control structures (total vs. partial composition control) are evaluated in Section 4. A class of simple composition control structures (single-composition control) are explored. Section 5 discusses the alternative of letting the reactor level uncontrolled, and Section 6 explores proportional only reactor level control as an alternative to feedforward control (feed ratio). Conclusions are drawn in Section 7.

2. Balanced scheme

A simple reactor/separator process is used to illustrate the control structure design (Papadourakis, Doherty, & Douglas, 1987). The process consists of a reactor and a distillation column in an interconnected structure as shown in Fig. 1 with all three compositions controlled

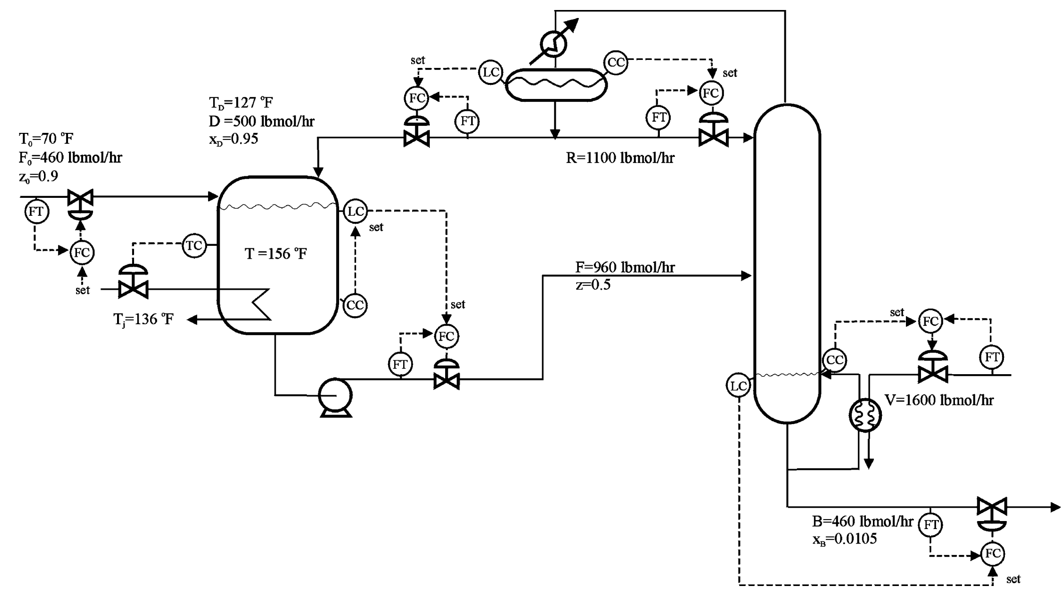

Fig. 1. Reactor/separator process with full composition control structure (control structure B-3: control x_B, x_D, and z).

(denoted as control structure B-3). The reaction is irreversible, $\mathscr{A} \rightarrow \mathscr{B}$, with first-order kinetics.

$$\mathscr{R} = kV_R z \tag{1}$$

where $\mathscr{R}$ is the reaction rate, k is the rate constant, V_R is the reactor holdup and z is the concentration of the reactant $\mathscr{A}$. The rate constant (k) is a function of temperature described by the Arrhenius expression. The reaction is exothermic, and the reactor temperature (T) is controlled by manipulating cooling water flow rate. The effluent of the reactor, a mixture of $\mathscr{A}$ and $\mathscr{B}$, is fed into a 20-tray distillation column. The product B is removed from the bottom of the column. The purified reactant $\mathscr{A}$ is the distillate product and is recycled back to the reactor. The column has a partial reboiler and a total condenser. The relative volatility between $\mathscr{A}$ and $\mathscr{B}$ is two. The recycle ratio (*recycle/fresh feed* $= RR = D/F_0 = D/B$) is approximately 1. Table 1 gives the nominal operating conditions for the process (Wu and Yu, 1996).

2.1. Snowball effects

From steady-state material balances, we have:
Reactor:

$$F_0 + D = F \tag{2}$$
$$F_0 z_0 + Dx_D = Fz + V_R kz \tag{3}$$

Column:

$$F = D + B \tag{4}$$
$$Fz = Dx_D + Bx_B \tag{5}$$

Notice that external flows in and out of the system are the reactor fresh feed flow rate (F_0) and the column bottoms flow rate (B), respectively. Rearranging Eqs. (2)–(5), we have:

Table 1
Steady-state parameters for reactor/separator system

Fresh feed flow rate (F_0)	460.0 (lbmol/h)
Fresh feed composition (z_0)	0.9 (mole fraction)
Fresh feed temperature (T_0)	70.0 (F)
Reactor holdup (V_R)	2400.0 (lbmol)
Reactor temperature (T)	156.4 (F)
Reactor jacket temperature (T_j)	136.1 (F)
Activation energy (E)	30 841.0 (Btu/lbmol)
Pre-exponential factor (k_0)	2.297×10^{10} (/h)
Rate constant at steady-state temperature	0.33 (/h)
Overall heat transfer coefficient	150.5 (Btu/h/ft F)
Heat transfer area	3206.8 (ft^2)
Heat capacity	0.7 ($Btu/lb_m/F$)
Heat of reaction	−30 000 (Btu/lbmol)
Density in reactor	60.05 (lb_m/lbmol)
Column feed flow rate (F)	960.4 (lbmol/h)
Column feed composition (z)	0.5 (mole fraction)
Distillate flow rate (D)	500.4 (lbmol/h)
Distillate composition (x_D)	0.95 (mole fraction)
Reflux flow rate (R)	1100.0 (lbmol/h)
Bottoms flow rate (B)	460.0 (lbmol/h)
Bottoms composition (x_B)	0.0105 (mole fraction)
Vapor boilup (V)	1600.4 (lbmol/h)
Number of trays	20
Feed tray	12
Relative volatility	2
Liquid hydraulic time constant	4 (s)
Recycle ratio (RR)	1.09

$$B = \frac{kV_R}{(z_0 - x_B)} \frac{x_B + x_D RR}{1 + RR} = \frac{kV_R}{(z_0 - x_B)} z \tag{6}$$

where RR is the *recycle ratio*, i.e., $RR = D/B$. Eq. (6) relates the production rate B to three compositions (z_0, x_D, and x_B) and three important operating variables (k, V_R and RR). Note that production rate, B, in Eq. (6) is equal to the total reaction rate, $\mathscr{R}$, divided by $(z_0 - x_B)$

(i.e., all $\mathscr{B}$ forms from the reaction and from the fresh feed as impurity). Assuming perfect separation and pure raw material (i.e., $x_D \to 1$, $x_B \to 0$ and $z_0 \to 1$) Eq. (6) becomes:

$$B = kV_R \frac{RR}{1 + RR} \tag{7}$$

Eq. (7) clearly indicates the production rate is affected by the reaction rate constant (k), reactor holdup (V_R) and the recycle ratio (RR, because this changes reactor composition). The conventional practice of holding reactor temperature and reactor holdup constant leaves us with only one variable to handle production rate changes: the recycle ratio. Since RR appears in both the numerator and denominator of Eq. (7), a large change in RR can only result in small change in the production rate. This is exactly what causes the 'snowball effect'. Furthermore, the effect can become very severe for recycle systems with a large recycle ratio, e.g., $RR > 5$. Eq. (7) offers useful insight into the process design as well as control of recycle processes. Despite the fact that this ''snowballing' can be alleviated by decreasing the one-pass conversion, equivalently z and RR (Eqs. (1) and (7)), it is sometimes unavoidable especially for highly exothermic reaction. Alternative control structures can be devised to overcome the snowball effect. One is the variable holdup strategies (Luyben, 1994; Wu and Yu, 1996) and the other is the variable temperature practice. The former is employed for the subsequent study since variation of reactor temperature is often limited by catalyst conditions, undesirable side reactions, materials of construction, maximum pressure etc. Notice that these alternatives may not be economically optimal (Skogestad, 2000), but they provide good disturbance attenuation as will be shown later.

2.2. Principle

The basic idea of the balanced scheme proposed by Wu and Yu (1996) is to distribute the work evenly among process units as the production rate changes. This leads to a practice similar to the *extensive* variable control of Georgakis (1986) in which intensive variables are kept constant at different operating conditions. Since the reactor temperature is held constant for the recycle process studied, obvious intensive variables are reactor composition (z) and distillate and bottoms compositions (x_D and x_B). Certainly, one can keep any three independent intensive variables constant. A straightforward approach is to control all three composition variables (z, x_D and x_B). Fig. 1 shows a possible control structure for the balanced scheme. This is a recycle process with a $R-V$ (reflux flow and vapor boilup) controlled distillation column and the reactor holdup is varied by the cascaded composition-to-level loops. Notice that this is just one possible control structure to keep the intensive variables constant. Despite the advantage of alleviating the snowball effect, three composition analyzers are required for this control structure. A question arises: do we really need three composition controllers to achieve the 'balance'? Steady-state disturbance analysis is useful in answering this question.

2.3. Steady-state disturbance analysis

The disturbance rejection capability of the balanced scheme can be analyzed using the disturbance sensitivity graph of Luyben (1975). The basic idea is to solve the steady-state component balances with z, x_D and x_B fixed as changes in the disturbance variables (F_0 and z_0) are made. The resulting required changes in the dependent variables (V_R, F, D, B, R and V) are examined to see what patterns result. Fig. 2A shows that by keeping z, x_D and x_B constant, the dependent variables (V_R, F, D, B, R and V) vary linearly with the same slope as the production rate (F_0) changes. All the dependent variables are expressed in the dimensionless from. It is important to note that the results, Fig. 2, are obtained from solving the *nonlinear* material balances. That means the balanced scheme shows a linear characteristic in handling production rate changes for the nonlinear recycle plant. Therefore, if we express the dependent variables in terms of ratios (e.g., D/B, V_R/F_0 etc.), instead of flow rates, they should remain constant for feed flow disturbance. Fig. 2B clearly illustrate the constant ratio characteristic. Similar results can be obtained for the feed composition (z_0) disturbance (Fig. 3A).

Since the intensive variables are kept constant, the following relationships for the scaled dependent variables (V_R, F, D and B) can be established.

$$\left(\frac{\partial V_R^*}{\partial F_0^*}\right)_{z,x_D,x_B} = \left(\frac{\partial F^*}{\partial F_0^*}\right)_{z,x_D,x_B} = \left(\frac{\partial D^*}{\partial F_0^*}\right)_{z,x_D,x_B} = \left(\frac{\partial B^*}{\partial F_0^*}\right)_{z,x_D,x_B} = 1 \tag{8}$$

where $y^* = (y - \bar{y})/\bar{y}$ and the overbar stands for nominal steady state. Similarly, the two internal flows (R and V) with feed flow rate disturbances become:

$$\left(\frac{\partial R^*}{\partial F_0^*}\right)_{z,x_D,x_B} = \left(\frac{\partial V^*}{\partial F_0^*}\right)_{z,x_D,x_B} = 1 \tag{9}$$

Similarly, for feed composition disturbance, from Eqs. (3) and (5):

$$\left(\frac{\partial V_R}{\partial z_0}\right)_{z,x_D,x_B} = \frac{\bar{F}_0}{\bar{k}\bar{z}} = \frac{\bar{V}_R}{\bar{z}_0 - \bar{x}_B}$$

Therefore, we have:

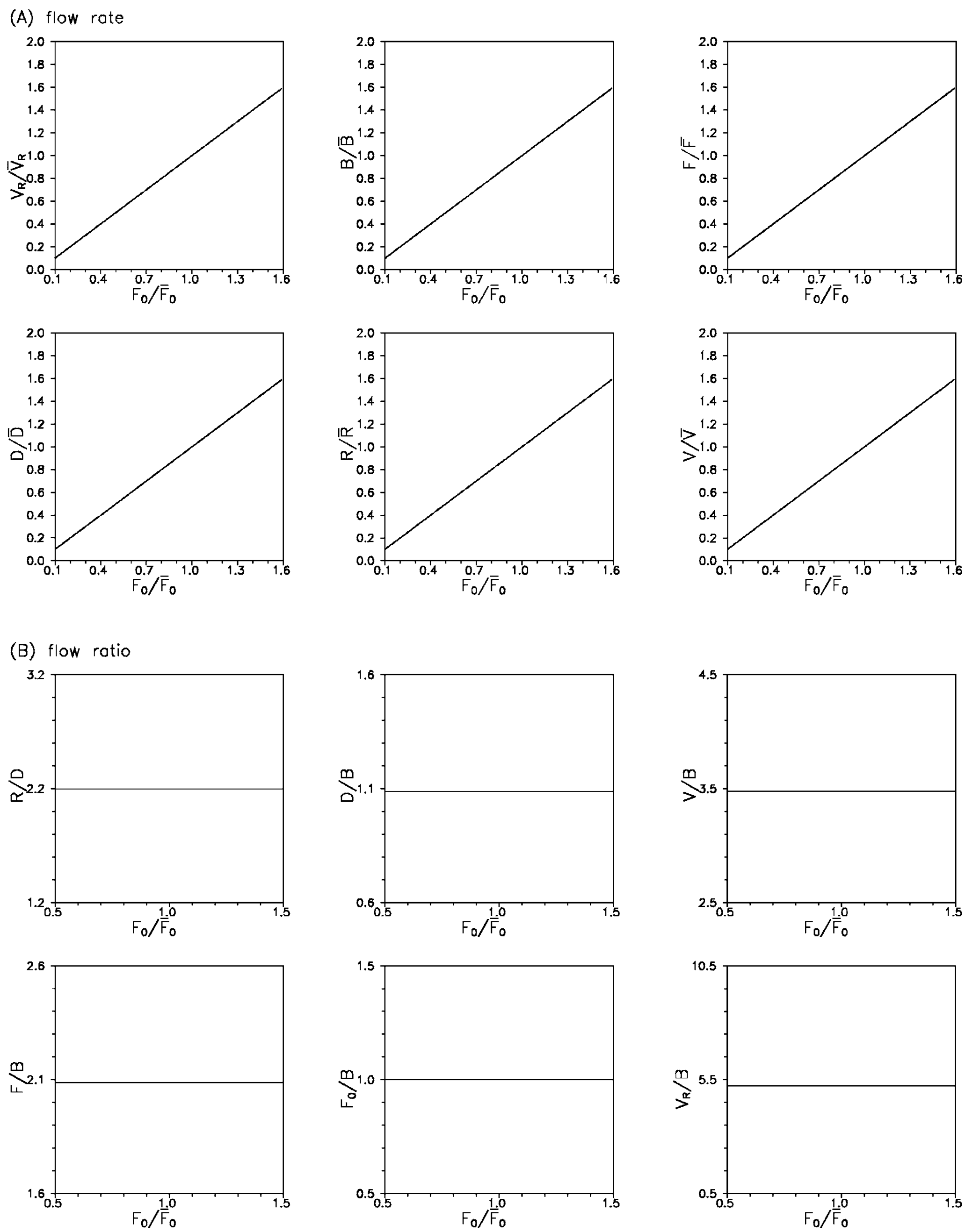

Fig. 2. Steady-state values of (A) flow rates and (B) flow rates for balanced scheme with feed flow disturbances.

$$\left(\frac{\partial V_R^*}{\partial z_0}\right)_{z,x_D,x_B} = \frac{1}{\bar{z}_0 - \bar{x}_B}$$

Disturbance analysis gives the relationship between the manipulated inputs and load variables while keeping controlled variables constant, i.e., $(\partial u^*/\partial d^*)_{y^*}$ where d is disturbance variables. For the balanced scheme, we have:

$$\begin{bmatrix} V_R^* \\ F^* \\ D^* \\ B^* \\ R^* \\ V^* \end{bmatrix} = \begin{bmatrix} 1 & \dfrac{1}{\bar{z}_0 - \bar{x}_B} \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} F_0^* \\ z_0 \end{bmatrix} \qquad (10)$$

The matrix in Eq. (10) is denoted as the disturbance

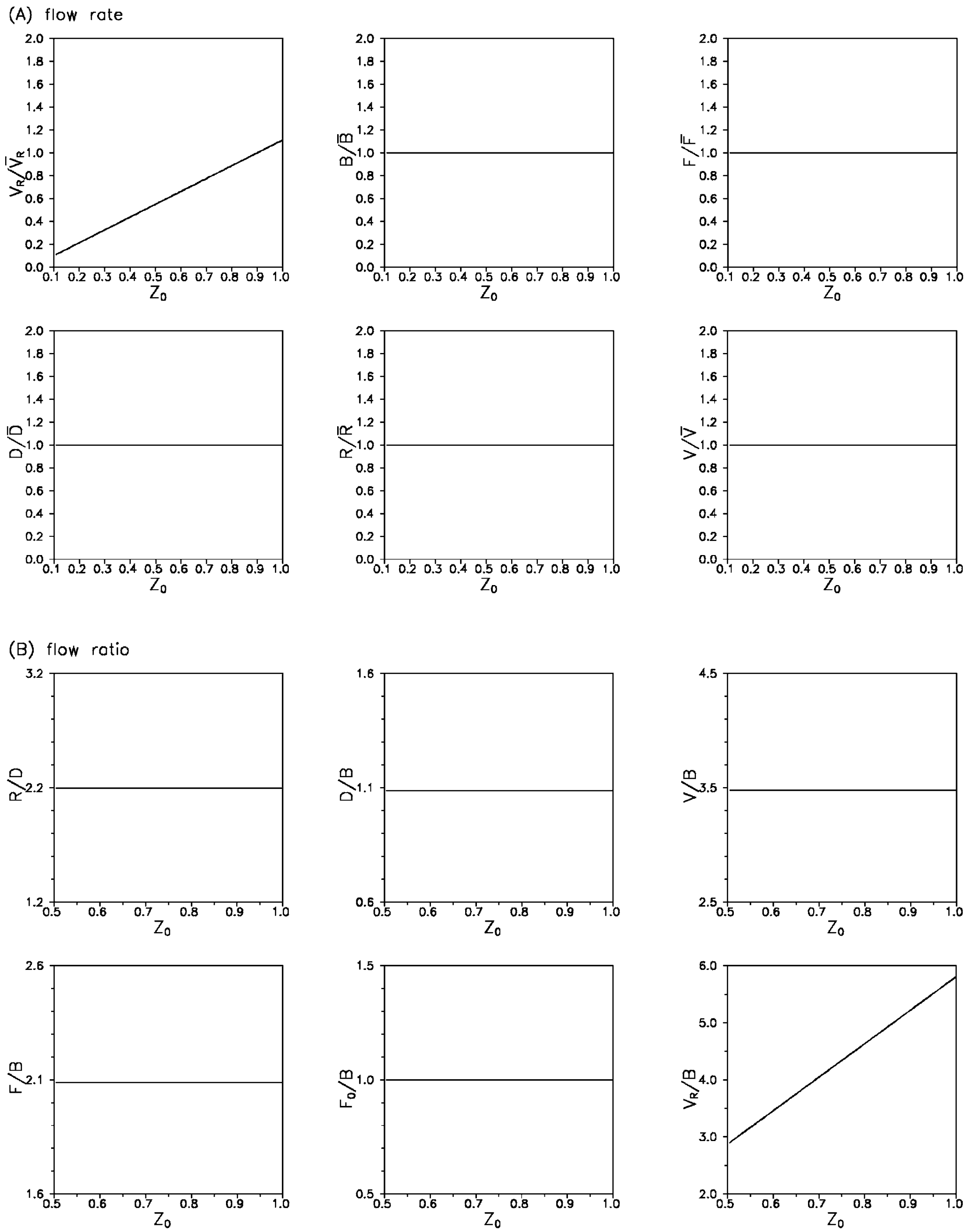

Fig. 3. Steady-state values of (A) flow rates and (B) flow ratios for balanced scheme with feed composition disturbances.

sensitivity matrix hereafter. This is the steady-state information we need to help in the design of control structures. It should be noted that Eq. (10) gives the exact relationship (not the linearized result) between the inputs and loads.

3. Control structure design

The essence of the balanced scheme is to maintain constant compositions in the face of major disturbances. In doing this, the ‘snowball’ effect can be eliminated as shown in Figs. 2 and 3. But do we need all three composition loops?

3.1. Full control (B-3)

If simple flow rates are used as manipulated variables, we are left with no option but to control all three composition variables. The reason is that the disturbance sensitivity matrix shows non-zero gains between the inputs and feed flow disturbance (first column of disturbance sensitivity matrix in Eq. (10)). Composition controllers can be employed to bring the manipulated inputs to the desired steady-state values in order to reject the disturbance. Fig. 1 shows that F, D and B are used for inventory control and V_R, R and V are employed for composition control. In terms of distillation control, this is a $R-V$ controlled column. Note that this is not the only option for full control. Different configurations such as $D-V$ structure can be used for dual composition control.

3.2. Partial control: two composition loops (B-2)

The concept of partial control (Skogestad & Postlethwaite, 1996; Luyben et al., 1999) is useful in simplifying the control structures. The control objective is to eliminate some of the composition loops. Eq. (10) offers insight into how to achieve this. For feed flow disturbances, all flow rates vary with the same proportion. Therefore, variable transformation can be used to make the extensive variable *invariant* under load changes. A simple way to achieve this is to use ratio schemes.

If we do ratio the reactor outflow (F) to the feed flow (F_0), disturbance sensitivity analysis gives:

$$\begin{bmatrix} V_R^* \\ (F/F_0)^* \\ D^* \\ B^* \\ R^* \\ V^* \end{bmatrix} = \begin{bmatrix} 1 & \dfrac{1}{\bar{z}_0 - \bar{x}_B} \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} F_0^* \\ z_0 \end{bmatrix} \tag{11}$$

The results (Eq. (11)Figs. 2B and 3B) show that the flow ratio F/F_0 has to be fixed in order to reject load disturbances. This is indicated by the second row in the disturbance sensitivity matrix. Therefore, instead of controlling all three compositions, we can keep all intensive variables constant by controlling one ratio (F/F_0) and two compositions. The two compositions can be x_D and x_B, z and x_B or z and x_D. One obvious choice is the product composition x_B, but the other one is less clear. As pointed out by Wu and Yu (1996), reactor composition (z) exhibits inverse response for V_R set point changes. Therefore, x_D is chosen as the second controlled variable. Fig. 4 shows that three inventories are controlled using D, R and B. The top composition x_D is maintained by changing the set point of the reactor holdup (V_R^{set}) and the product composition x_B is controlled in vapor boilup (V). This is the control structure proposed by Wu and Yu (1996), it is denoted as the B-2 structure.

Fig. 2B and 3B reveal that all the flow ratios are constant for both feed flow and feed composition disturbances in the balanced scheme. Therefore, the ratio scheme can be extended further to reduce the number of composition loops.

3.3. Partial control: one composition loop (B-1)

In order to simplify the control structure even further we have to make another *row* in the disturbance sensitivity matrix zero. An obvious choice is to use ratio control in the distillation column. For the control structure shown in Fig. 4, the boilup ratio (V/B) is a candidate manipulated variable. Following the transformation, the disturbance sensitivity matrix becomes:

$$\begin{bmatrix} V_R^* \\ (F/F_0)^* \\ (V/B)^* \\ D^* \\ B^* \\ R^* \end{bmatrix} = \begin{bmatrix} 1 & \dfrac{1}{\bar{z}_0 - \bar{x}_B} \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} F_0^* \\ z_0 \end{bmatrix} \tag{12}$$

The results imply we can drop another composition loop by keeping the second ratio (V/B) constant. That means by controlling one composition and two ratios, we can keep all the intensive variables constant at steady states. Three flow rates (D, B, and R) are used for inventory control (Eq. (12)), and two ratios are kept constant. Therefore, we are left with only one manipulated input, reactor holdup, for composition control.

In principle, controlling either one of these three compositions (z, x_D and x_B) can achieve the ‘balance’. As pointed earlier, x_D and x_B are two likely candidates. Fig. 5 shows the case when x_D is maintained by changing V_R^{set}, control structure B1. A more realistic approach is to control the product purity x_B. Fig. 6 shows a control scheme in which reactor holdup is selected to control x_B. This is denoted as the B-1a control structure hereafter.

The control scheme shown in Fig. 6 has some practical limitations, unfavorable dynamics between the manipulated and controlled variables. One alternative is to change the distillation control configuration to control x_B with reflux and distillate flow on the top level on, but, again, we have long delay in the composition loop. It would be better to control product quality x_B directly with column boilup V. This would give the minimum variability in product quality. Control schemes that employ this x_B-V loop are presented in a later section of this paper.

The next question naturally arises: can we eliminate all the composition loop from the control system? Eq. (12) shows that the only manipulated variable left for composition control is the reactor holdup V_R. Unfortunately, V_R gives different behavior for different types of disturbances, e.g., different values in the first row of the disturbance sensitivity matrix. Therefore, for the two major disturbances considered, we are not able to maintain the ‘balance’ without using at least one composition controller.

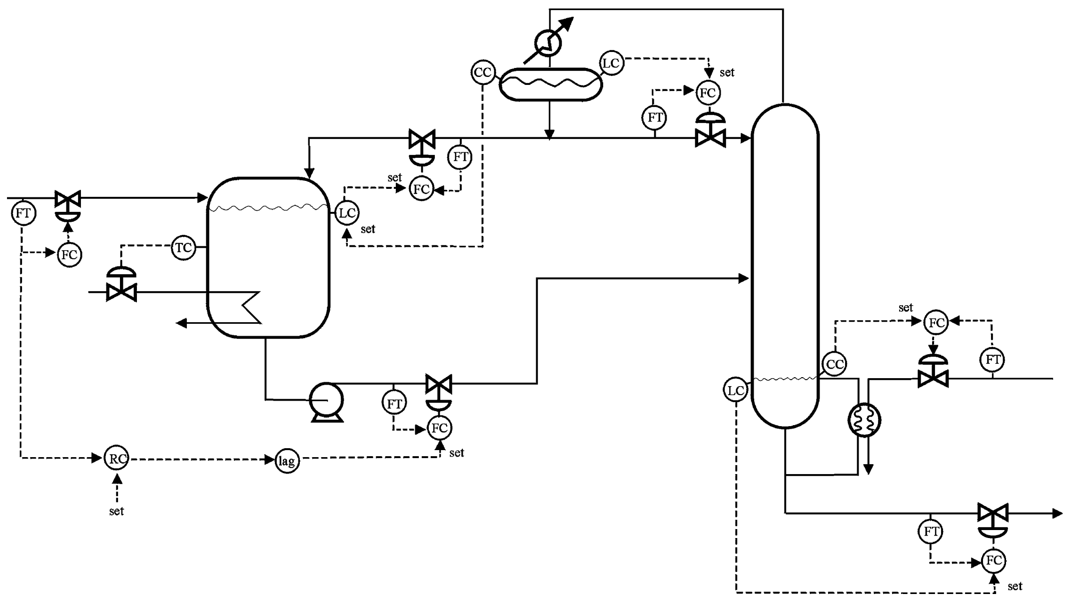

Fig. 4. Reactor/separator process with two composition loops (control structure B-2: control x_B, x_D, and F/F_0).

4. Total control vs partial control

The dynamics of the reactor/separator process are analyzed using a series of rigorous dynamic simulations. Parameters characterizing dynamic behavior, e.g., hold-ups in column and reactor, are taken from Wu and Yu (1996). Six minutes of analyzer dead time and one minute of temperature measurement lag are assumed in the composition and temperature loops, respectively.

4.1. Controller design

Unless otherwise mentioned, the same plantwide tuning procedure is applied to all control structures. The controller design is based on the plantwide tuning of Wu and Yu (1996). The tuning sequence starts from the inventory loops, then the feedforward controllers are designed and finally the composition loops are tuned. Proportional-only (P-only) level controllers are used for

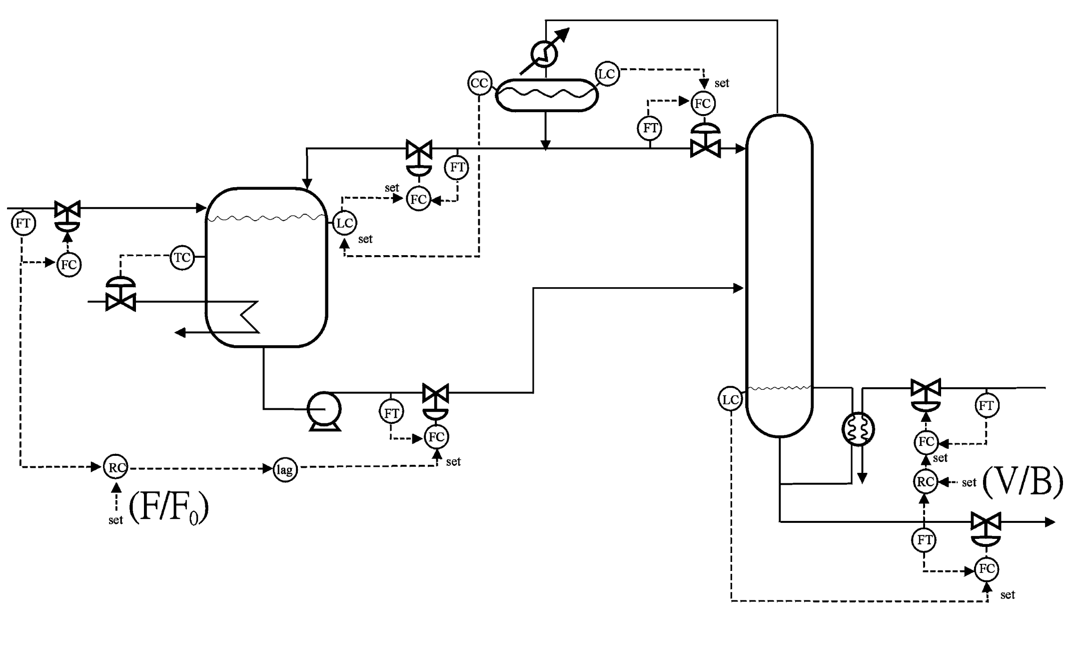

Fig. 5. Reactor/separator process with one composition loop (control structure B-1: control x_D, F/F_0, and V/B).

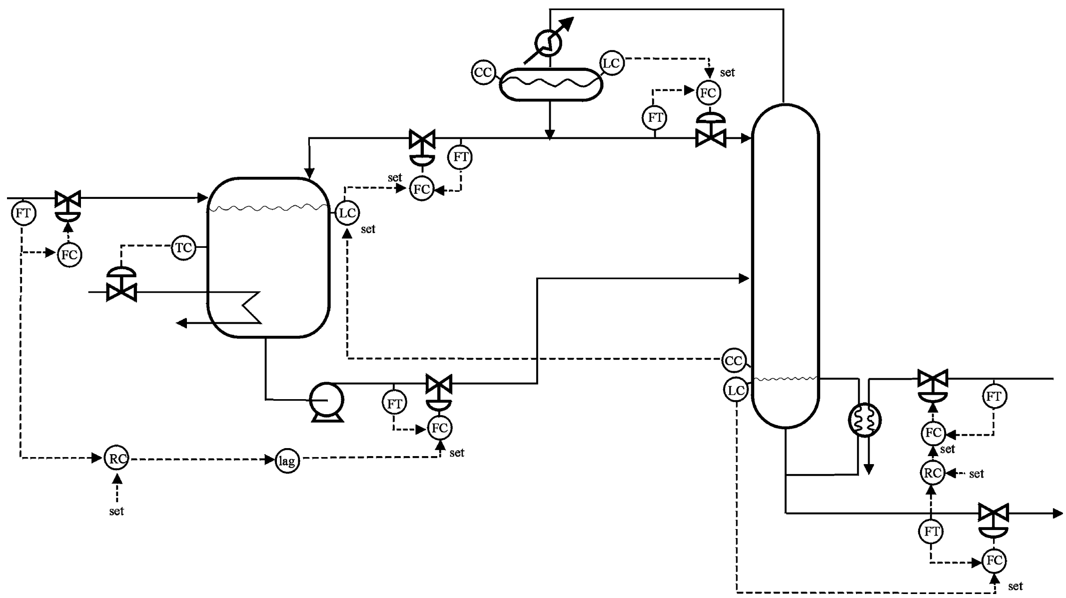

Fig. 6. Reactor/separator process with one composition loop (control structure B-1a: control x_B, F/F_0, and V/B).

top and bottoms levels of distillation column. The closed-loop time constants for the level loops in the distillation column are set to 50% of the residence times. Since the reactor level is cascaded by a composition loop, a P-only controller is employed for reactor level control. A tight reactor level control is tuned by setting the closed-loop time constant to be 3% of the residence time. Table 2 gives the tuning constant for the level loop. Since a ratio control is used, a dynamic element is placed in the F/F_0 feedforward path (Fig. 4). This 'lag' device with the time constant set to be 100% of the reactor residence time. The reason for the slow lag time constant is that we would like to withdraw the product $\mathscr{B}$ at a rate comparable the reaction rate. PI controllers are employed for quality control.

Temperature and composition loops are tuned using the multivariable autotuner of Shen and Yu (1994). The relay-feedback based autotuner performs the tuning sequentially, and the procedure is repeated until the corresponding tuning constants converge. Fig. 8 illustrates the tuning sequence of the full control structure. First, the relay feedback test is performed on the $T-T_j$

Table 2
Ultimate properties and controller parameters for different control structures

Structure	Parameter pairing	K_u [a]	P_u [b]	K_c [a]	τ_I [b]
B-3	Temperature loop $T-T_j$	16.98	4.0	5.66	8.0
	Composition loop x_B-V	−2.67	30.3	−0.89	60.6
	Composition loop x_D-R	0.84	40.2	0.28	80.4
	Composition loop $z-V_R^{set}$	−0.32	54.7	−0.11	109.4
	Level loop			−6.0	
B-2	Temperature loop $T-T_j$	17.0	4.0	5.67	8.03
	Composition loop x_B-V	−4.38	22.4	−1.46	44.7
	Composition loop $x_D-V_R^{set}$	−0.14	32.0	−0.05	63.9
	Level loop			6.1	
B-1a	Temperature loop $T-T_j$	17.06	4.0	5.69	8.0
	Composition loop $x_D-V_R^{set}$	−1.37	26.0	−0.46	52.0
	Level loop			6.1	
B-1b	Temperature loop $T-T_j$	17.0	4.02	5.672	8.04
	Composition loop $x_B-V_R^{set}$	−8.58	37.65	−2.86	75.3
B-1c	Temperature loop $T-T_j$	17.07	4.0	5.69	8.0
	Composition loop $x_B-V_R^{set}$	−8.58	37.6	−2.87	75.2
	Level loop			−1	

[a] Transmitter spans: x_D, x_B: 0.1 mole fraction; z: 0.2 mole fraction; level: twice nominal steady-state holdup; valve gains: twice nominal steady-state flow rate except for fresh feed flow (three times nominal steady-state flow rate).
[b] Minimum.

loop and ultimate gain K_u and ultimate period (P_u) can be found from system responses. Once K_u and P_u are available, K_c and τ_I can be found according to:

$$K_c = \frac{K_u}{3} \tag{13}$$

$$\tau_I = 2P_u \tag{14}$$

Next, the x_B–V loop is relay feedback tested with the T–T_j loop on automatic. The procedure is repeated for x_D–R and z–F loops. Fig. 7 shows that this procedure is repeated for another round to ensure that these parameters really converge. Table 2 gives the tuning constants for the quality loops.

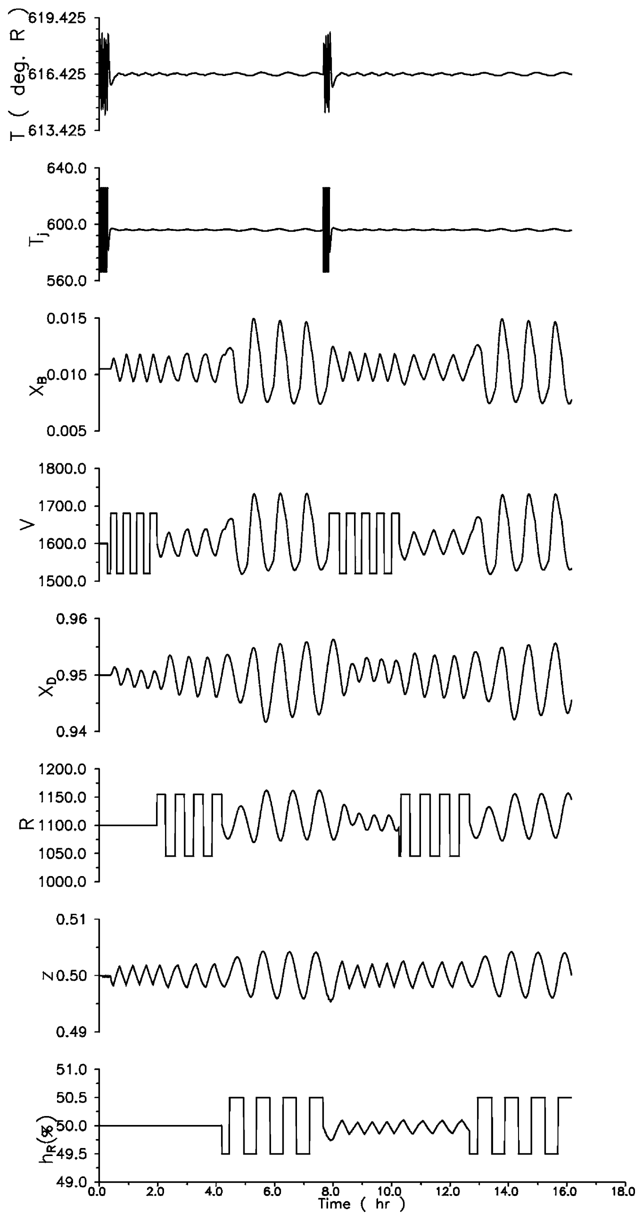

Fig. 7. Autotuning of the T–T_j, x_B–V, x_D–R and z–h_R^{set} loops for control structure B-3.

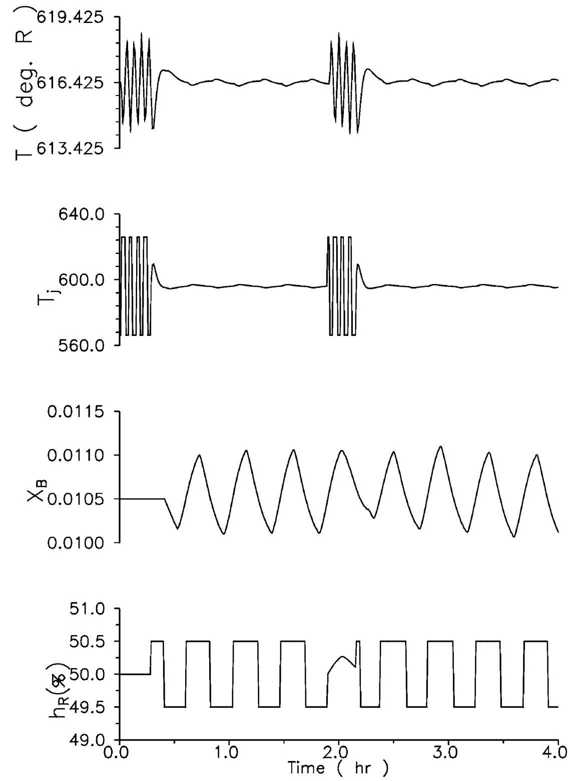

Fig. 8. Autotuning of the T–T_j, and x_B–h_R^{set} loops for control structure B-1.

It takes 16 h to complete the tuning for the B-3 control structure. However, Fig. 8 shows that for the simplest control structure, the tuning takes 4 h to complete. In addition to simpler instrumentation, the advantage of fewer composition loops is clearly demonstrated in the controller design phase.

4.2. Performance

Control structures with one, two and three composition loops are tested on the reactor/separator process by performing a series of nonlinear dynamic simulations. Figs. 9–11 show what happens when step changes are made in fresh feed flow rate for these three control structures. For the full control structure (B-3), as expected all three compositions return to set points after production rate changes (Fig. 9). For the partial control with two composition loops (B-2), Fig. 10 shows that all three compositions (z, x_D and x_B) again return to their nominal values. For the case of one composition loop (B-1a), the results show that the two uncontrolled compositions (z and x_D) return to their nominal values at about the same rate as in the other two cases. With respect to individual composition, x_D is better controlled using the B-3 control structure while x_B is better controlled using B-2 control structure. In general, all three control structures give comparable composition responses (Figs. 9–11). That implies partial controls

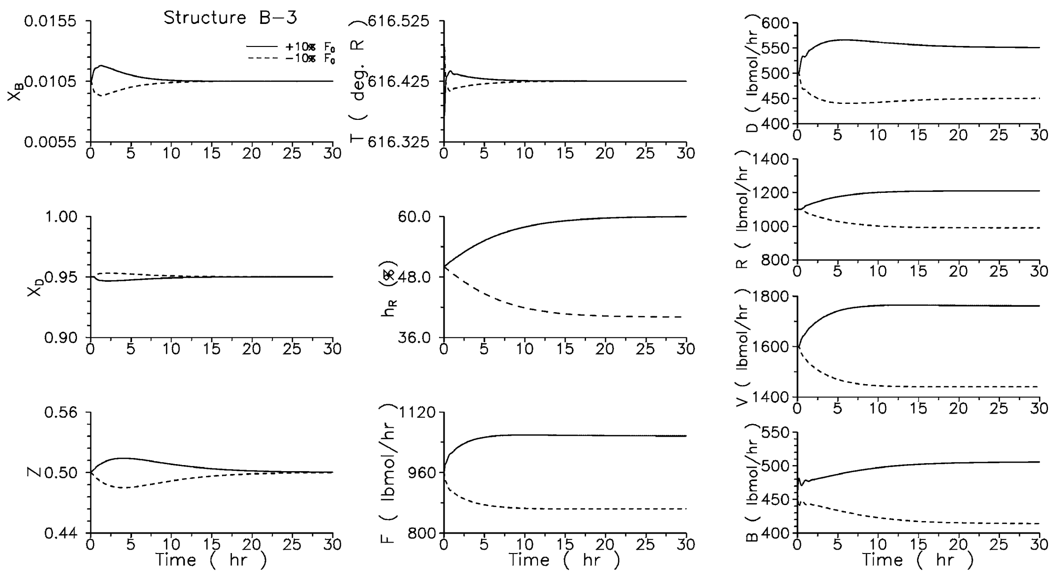

Fig. 9. Step responses of B-3 control structure for $\pm 10\%$ feed flow rate changes.

perform as well as full control. Similar results can be observed for feed composition disturbances as shown in Fig. 12.

4.3. Discussion

The control structure design procedure shows that only one composition loop is sufficient to return all three compositions to their the nominal values. This seems to be a simple and yet workable control structure, since we have an almost single-input–single-output system, i.e., one composition loops plus three level loops with two fixed flow ratios (Table 3). However, several drawback can be observed immediately. Since the control structure is derived from steady-state disturbance analysis, it is not exactly dynamically preferable. For example, we control the product composition by changing the reactor holdup. From the distillation control point of view, this is equivalent to controlling the product purity with feed composition, which may not be a good choice if alternatives exist. As pointed out earlier, it would be better to control x_B directly with vapor boilup. Next, the cascaded reactor level control results in poor flow transition as the production rate changes. That can be seen by analyzing the block diagram between F_0 and V_R. Time domain simulation, Fig. 11, shows that the manipulated variable (D) goes through an inverse response and the bottoms flow rate exhibits an unusual overshoot before reaching a new steady-state as the production rate changes. Internal

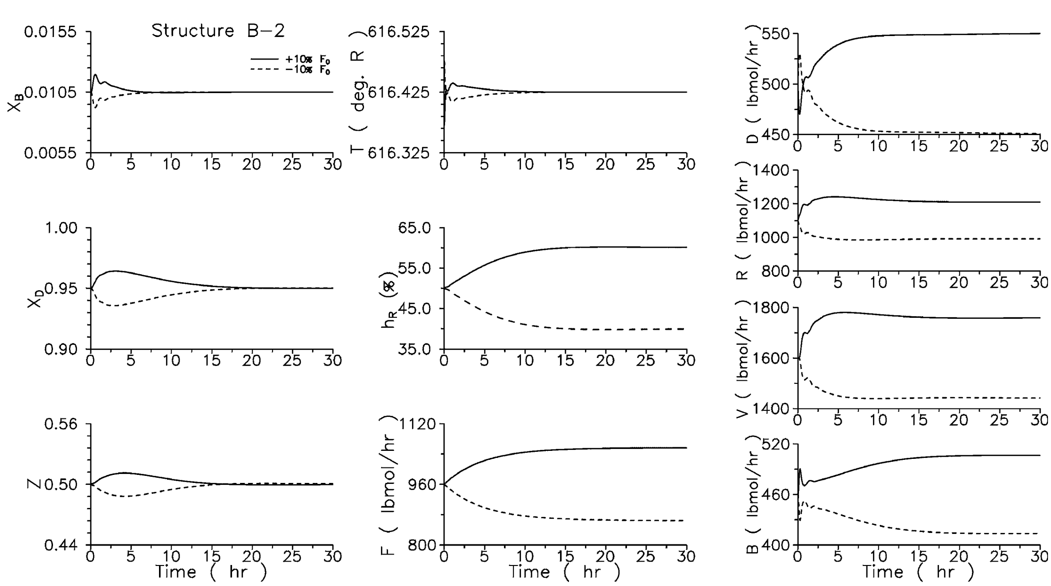

Fig. 10. Step responses of B-2 control structure for $\pm 10\%$ feed flow rate changes.

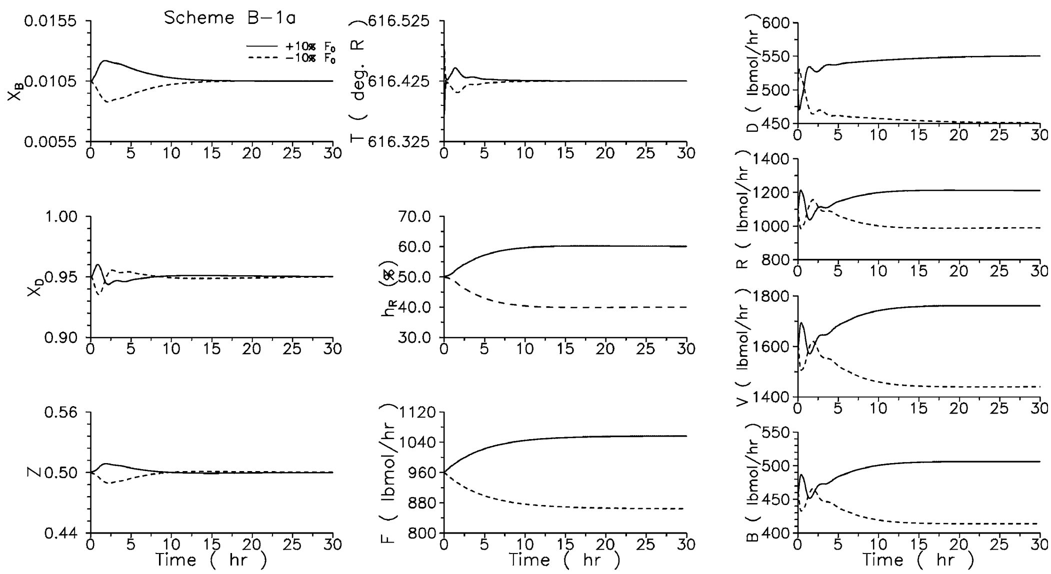

Fig. 11. Step responses of B-1a control structure for $\pm 10\%$ feed flow rate changes.

flows (R and V) in the distillation column are also perturbed in a similar manner.

5. Alternative 1: reactor level uncontrolled (B-1b)

5.1. Concept

It is well-known that reactor control, reaction rate control in particular, constitutes one of the most important factor in plantwide control. It seems natural to control reactor temperature, reactor level and/or reactor composition. However, for the balanced control structure, we are controlling two flow ratios and one composition. This leads to a self-regulating reactor level.

Fig. 13 shows a simplified flow/inventory configuration of the recycle plant. For six possible flow rates, we have only three degrees of freedom. F_0 is used to set the production rate and we are left with two degrees of freedom. Once any two flow ratios are fixed, the rest of the flows settle to their desired values. For example, if we set the feed ratio (FR) and the boilup ratio (BR), this results in a constant recycle ratio (RR) and reflux ratio (rR) (Fig. 13). This implies that we *automatically* have a two-ratio scheme (rR–BR), or the Ryskamp scheme, for distillation control. Since we are controlling one composition and fixing two ratios, the degrees of freedom analysis for the distillation column indicates that the other two compositions must be held at their steady-state values. That explains why the one-composition-

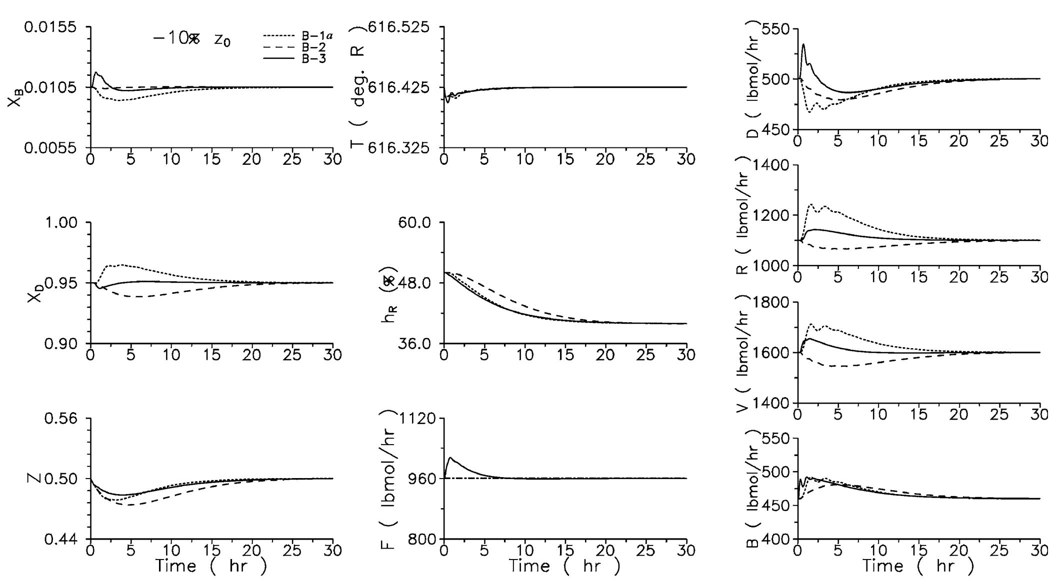

Fig. 12. Step responses of control structures B-3, B-2, and B-1a for a -10% feed flow rate change.

Table 3
Balanced control structures with different level of complexity in composition controls

Structure	Controlled			Remarks
B-3 (Fig. 1)	x_B	x_D	z	Control all three compositions
B-2 (Fig. 4)	x_B	x_D	F/F_0	Control two compositions and one ratio
B-1 (Fig. 5)	V/B	x_D	F/F_0	Product composition x_B is not controlled
B-1a (Fig. 6)	x_B	V/B	F/F_0	Poor control of x_B due to slow dynamics
B-1b (Fig. 7)	x_B	R/D	F/F_0	Reactor level not controlled
B-1c (Fig. 21)	x_B	R/D	V_R/F	P-only control of reactor level with K_c equal to the inverse of the residence time (Eq. (27))

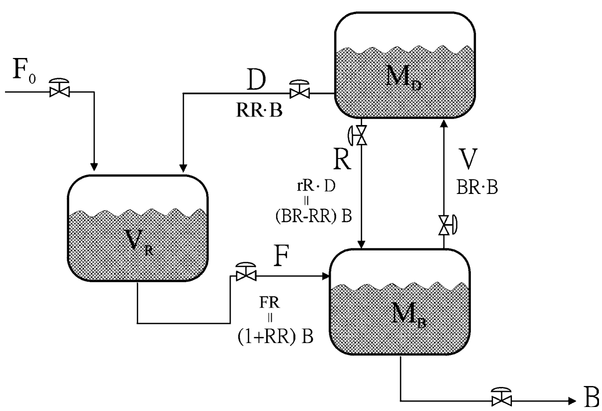

Fig. 13. Simplified flow/inventory configuration for the reactor/separator process.

two-ratio control structure results in error-free control in all three compositions. More importantly, Eq. (1) reveals that the reactor level has to change to a new steady-state value as the production rate changes. This can also be derived analytically from balance equations. Component material balance around the reactor (Fig. 6) gives:

$$\frac{\mathrm{d}V_R z}{\mathrm{d}t} = F_0 z_0 + D x_D - k V_R z - F z \tag{15}$$

Since two flow ratios are fixed, Eq. (15) can be rewritten as (Fig. 13):

$$\frac{\mathrm{d}V_R z}{\mathrm{d}t} = F_0[z_0 + RR x_D - (1 + RR) z] - k V_R z \tag{16}$$

The balanced scheme leads to constant column feed and distillate compositions (z and x_D). Therefore, with this constant composition assumption, we have:

$$\bar{z}\frac{\mathrm{d}V_R}{\mathrm{d}t} = F_0[\bar{z}_0 + \bar{R}R\bar{x}_D - (1 + \overline{RR})\bar{z}] - \bar{k} V_R \bar{z} \tag{17}$$

where the overbar denotes nominal steady-state value. After some algebraic manipulation, the result of Laplace transformation gives:

$$\left(\frac{V_R}{F_0}\right) = \frac{\left(\frac{1}{\bar{k}}\right)\left[\frac{(\bar{z}_0 - \bar{z}) + (\bar{x}_D - \bar{z})\bar{R}R}{\bar{z}}\right]}{\left(\frac{1}{\bar{k}}\right)s + 1} \tag{18}$$

Eq. (18) clearly indicates that the reactor holdup goes through a first order response with a time constant of $(1/\bar{k})$. Therefore, for the one-composition-two-ratio control structure, the reactor level exhibits self-regulating behavior. That indicates that we do not have to control the reactor level. This is no surprise since V_R has a steady-state effect and this applies to control structures in Figs. 4–6.

If the reactor level is left uncontrolled, we have one more handle for control structure design (e.g., the distillate flow). Another advantage is that we can use the vapor boilup or the boilup ratio to control x_B instead of V_R^{set}. Therefore, the control structure B-1a is modified to (Fig. 14):

1) The fresh feed is flow controlled.
2) The reactor effluent is ratioed to the fresh feed.
3) The reflux ratio (rR) is fixed.
4) Only two liquid levels are controlled. The reflux drum level is maintained by changing the reflux flow and the base level is controlled by adjusting the bottoms flow.
5) The reactor temperature is controlled by the cooling water flow.
6) The bottoms composition (x_B) is controlled by changing the boilup ratio (BR).

This B-1b control structure consists of one composition loop and two level loops with two constant flow ratios. This structure is even simpler than the B-1a structure. Table 3 compares the control loops in these two structures.

5.2. Analyses

Since the dynamics of the reactor temperature is almost one order of magnitude faster than that of bottoms composition, the system is treated as a SISO system. Therefore, throughout the identification steps, the reactor temperature controller is set on the auto-

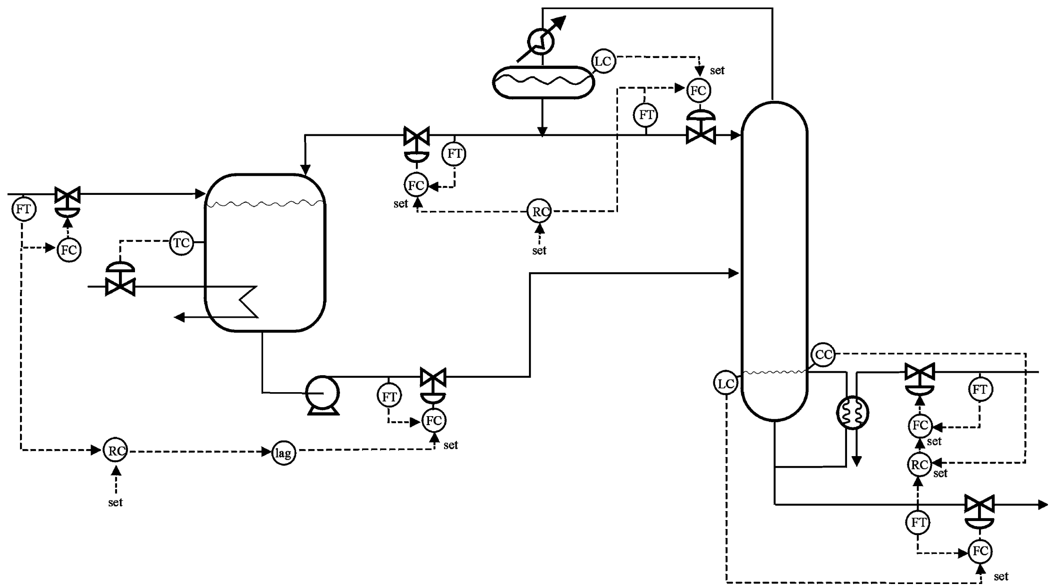

Fig. 14. B-1b control structure (control x_B R/D, and F/F_0).

matic mode. The combination of step test and relay feedback test (Luyben & Luyben, 1997; Yu, 1999) is used to identify the process transfer functions.

For the B-1a control structure, the step test reveals that x_B exhibits a lead/lag type of responses (Chang, Yu, & Chien, 1997), i.e., a fast jump is x_B followed by a slow dynamics. The process gain is obtained from steady-state simulation and the dead time is read off from step test. After assuming a lead time constant, two process time constants are calculated from the results of a relay feedback test. The ultimate gain and ultimate period are: $K_u = -1.37$ and $P_u = 26$ h (Table 2). Table 4 gives the process transfer functions. For the B-1b structure, Fig. 15 shows that we have an integrating system behavior for a 10% step increase in the boilup ratio (BR). Actually, it is not hard to understand the unexpected responses. While fixing F_0, we have only two degrees of freedom for the flow. In this structure, we already fix the feed ratio (FR) and reflux ratio (rR) and a step change in BR offsets the flow balance and, subsequently, leads to instability is the reactor level. Following notations in Fig. 13, the material balance around the reactor gives (Fig. 13):

$$\frac{dV_R}{dt} = F_0 + D - F$$

$$= \left(1 + \frac{BR}{1 + rR}\right)F_0 - FRF_0 \tag{19}$$

where V_R is the reactor holdup. When the feed ratio and reflux ratio are fixed, a change in the boilup ratio gives:

Table 4
Process and load transfer functions for B-1a, B-1b and B-1c control structures

	Process	Load	
B-1a	$\frac{x_B}{V_R^{set}} = \frac{-3.98(0.1s+1)e^{-0.1s}}{(0.146s+1)(0.078s+1)}$	$\frac{x_B}{F_0} = \frac{3.9836e^{-0.8s}}{0.07s^2+0.468s+1}$	$\frac{x_B}{Z_0} = \frac{0.4476e^{-1.5s}}{(10.658s)(0.181s+1)}$
B-1b	$\frac{x_B}{BR} = \frac{-104.98e^{-0.09s}}{s(2.11s+1)}$	$\frac{x_B}{F_0} = \frac{0.3524e^{-0.8s}}{0.31s^2+0.96s+1}$	$\frac{x_B}{z_0} = \frac{0.4476e^{-1.5s}}{(10.658s+1)(0.181s+1)}$
B-1c	$\frac{x_B}{BR} = \frac{-9.07e^{-0.1s}}{2.97s+1}$	$\frac{x_B}{F_0} = \frac{9.32e^{-0.8s}}{0.304s^2+0.55s+1}$	$\frac{x_B}{z_0} = \frac{0.4476e^{-1.5s}}{(10.658s+1)(0.181s+1)}$

* Transmitter spans: $x_B = 0.1$ mole fraction; $z_0 = 0.2$ mole fraction; BR = four times of nominal value; ** Valve gains: twice nominal steady-state flow rate except for fresh feed flow (three times nominal steady-state flow rate).

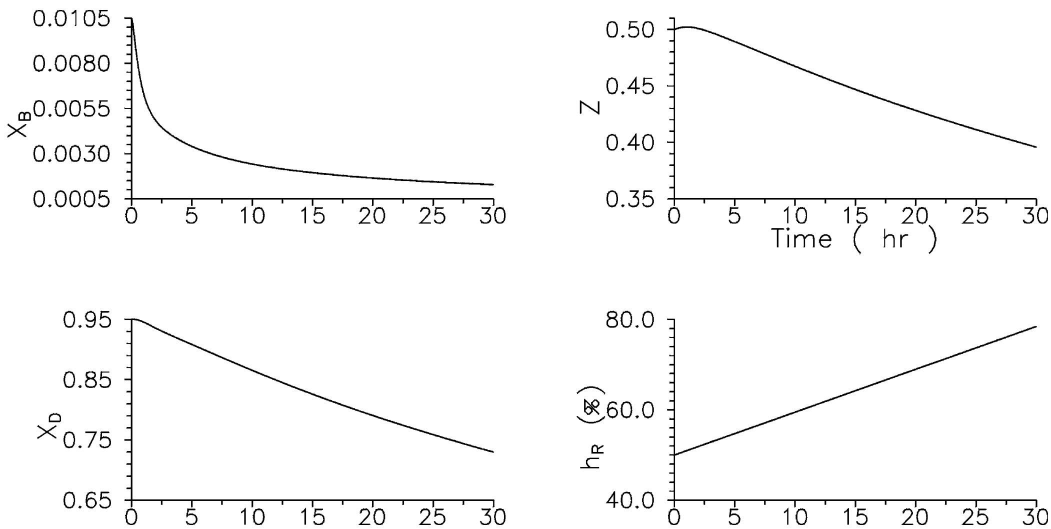

Fig. 15. Step responses of B-1b control structure for a 10% increase in boilup ratio (BR).

$$\frac{dV_R}{dt} = (1 + \overline{rR} + BR)\bar{F}_0 - (1 + \overline{rR} + \overline{BR})\bar{F}_0$$
$$= \frac{BR - \overline{BR}}{1 + \overline{rR}}\bar{F}_0 \tag{20}$$

where the overbar stands for the steady-state value. The result of Laplace transformation shows the integrating behavior.

$$\left(\frac{V_R}{BR}\right) = \frac{\bar{F}_0}{s} \tag{21}$$

Recognizing this fact, an integrator is added to the process transfer function between x_B and BR. Therefore, two parameters, lag time constant and dead time, can be calculated from the relay feedback test. Table 4 gives the process transfer function (G) for the B-1b structure. Notice that the ultimate period, $P_u = 37.6$ h, is much larger than that of the B-1a structure. That means at least from the process transfer function point of view, we do not have as favorable dynamics for the B-1b control structure as one would assume intuitively.

A similar approach is taken to find load transfer functions. For a step increase in the fresh feed flow, both control structures show underdamped responses for the bottoms composition (Fig. 16). Moreover, the steady-state disturbance gain for the B-1b structure is much smaller than that of the B-1a structure. That implies the B-1b control structure is a better choice in minimizing the propagation of flow disturbances in open-loop. For the B-1b structure, feed flow disturbances simply ride through the process units without having much effect on compositions as shown in Fig. 16. Moreover, despite having slower dynamic responses, the B-1b structure

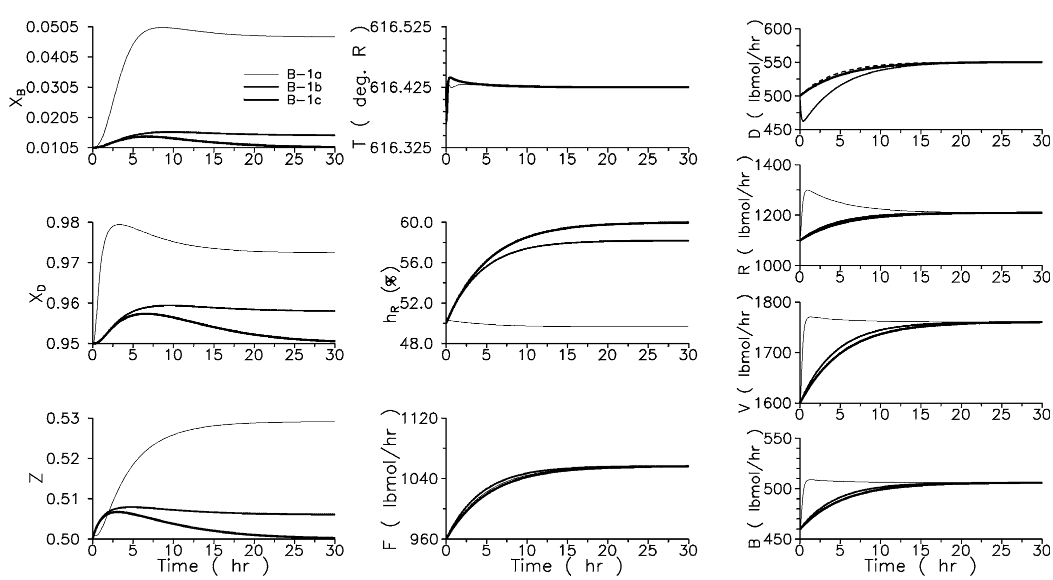

Fig. 16. Open-loop step responses of B-1a, B-1b, and B-1c control structures for a 10% increase in fresh feed flow rate.

shows a smoother flow transition as the production rate changes (Fig. 16). However, for feed composition disturbances, both control structures show exactly the same responses and, therefore, have the same load transfer function. That can be understood since these two structures differ from each other in the arrangement of inventory loops and flows are not disturbed by feed composition changes.

5.3. Results

Having all the transfer functions, we can analyze the disturbance rejection capabilities under closed-loop control. First, the composition controller is autotuned from relay feedback tests. For the PI controller, the controller gain is set to one-third of the ultimate gain (K_u) and the reset time is tuned to be twice of the ultimate period (P_u). Table 2 also gives controller parameters for the B-1b structure. The closed-loop load transfer function ($G_{L,CL}$) is used to evaluate disturbance rejection of the corresponding control structure with the composition loop closed. Block diagram of the closed-loop system gives the following load transfer function:

$$G_{L,CL} = \frac{G_L}{1 + GK} \tag{22}$$

where G and G_L are the process and load transfer functions, respectively, and K is the controller transfer function. As expected, Fig. 17 shows that, for the feed flow disturbance, the B-1b structure has a much better disturbance rejection capability than the B-1a control structure. For feed composition disturbances, Fig. 18 indicates that the B-1b structure shows a better disturbance rejection at low frequency range and the performance at high frequencies is about the same. The improved disturbance rejection comes from the wider bandwidth of '$(1 + GK)(i\omega)$' for the B-1b structure, since we have exactly the same G_L for feed composition changes.

The B-1b structure is compared to the B-1a structure using nonlinear rigorous dynamic simulations. Figs. 11 and 19 show what happens when $\pm 10\%$ step changes are made in the fresh feed flow rate. The results show that the B-1b control structure gives much better products composition (x_B) control. Moreover, rather smooth production rate (B) changes are observed for the B-1b structure. For the feed composition disturbance, again, the B-1b control structure gives better composition control. But the margin of improvement is not quite as large as the flow rate disturbances.

In practice, it may be difficult to accept the fact that we need *not* controlling the reactor level. This can be overcome by implementing override control. One straightforward approach is to override the reactor effluent flow by high or low reactor level.

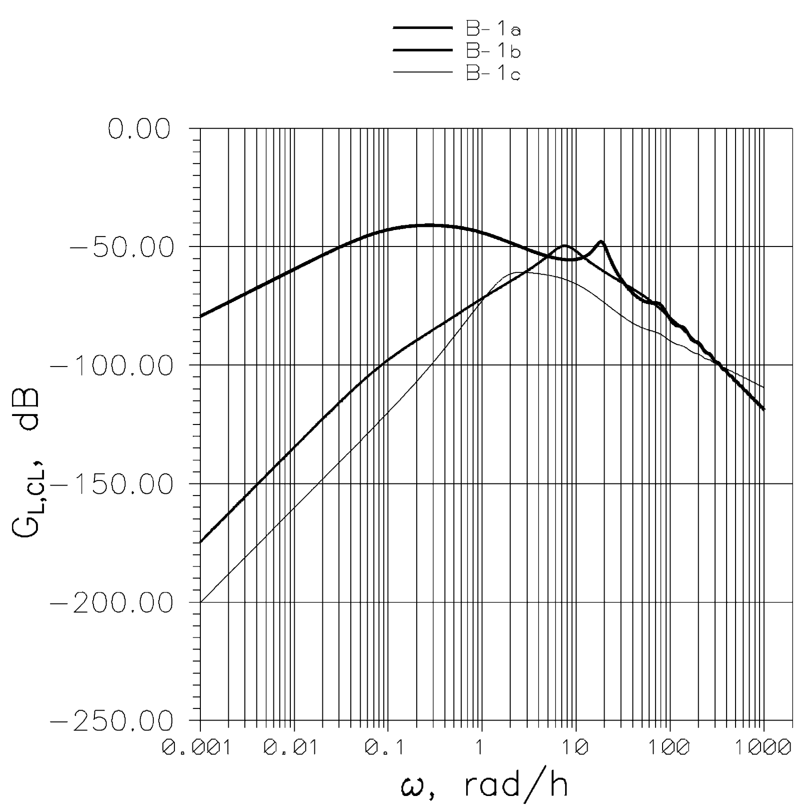

Fig. 17. Frequency responses of closed-loop load transfer function for feed flow disturbance.

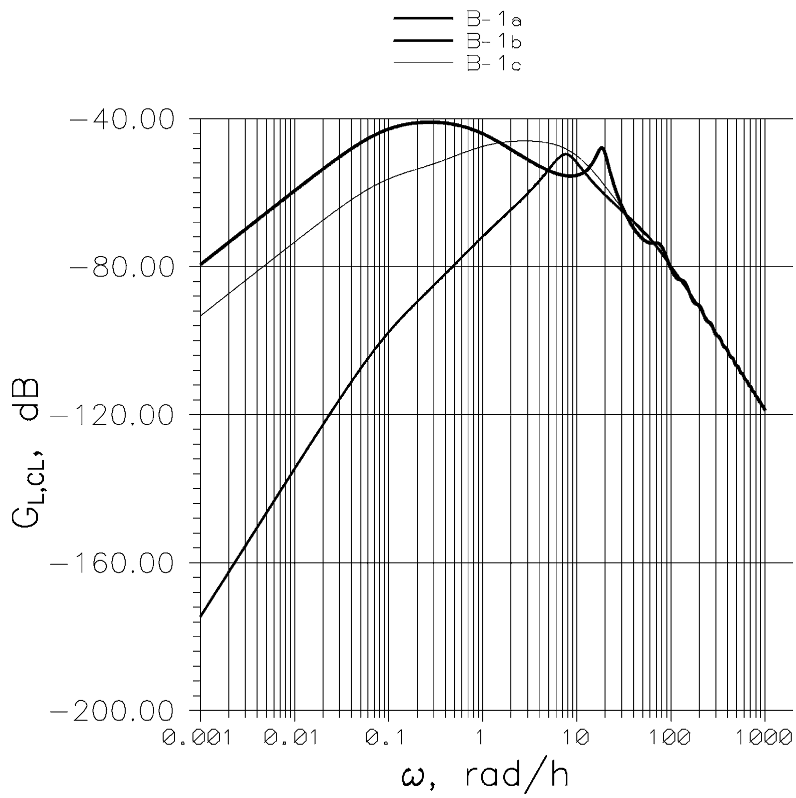

Fig. 18. Frequency responses of closed-loop load transfer function for feed composition disturbance.

6. Alternative 2: P-only reactor level control (B-1c)

6.1. Concept

In the B-1b control structure, a feedforward controller (Fig. 14) is designed to regulate the reactor effluent flow rate. In doing this, the reactor level floats to a desired steady state as a new production rate is set. The reason is obvious: we would like to maintain a constant reactor residence time (τ_{res}). τ_{res} is defined as:

$$\tau_{res} = \frac{\bar{V}_R}{\bar{F}} \tag{23}$$

A P-only reactor level controller can achieve the same without fixing the flow ratio (Fig. 21). Actually we are

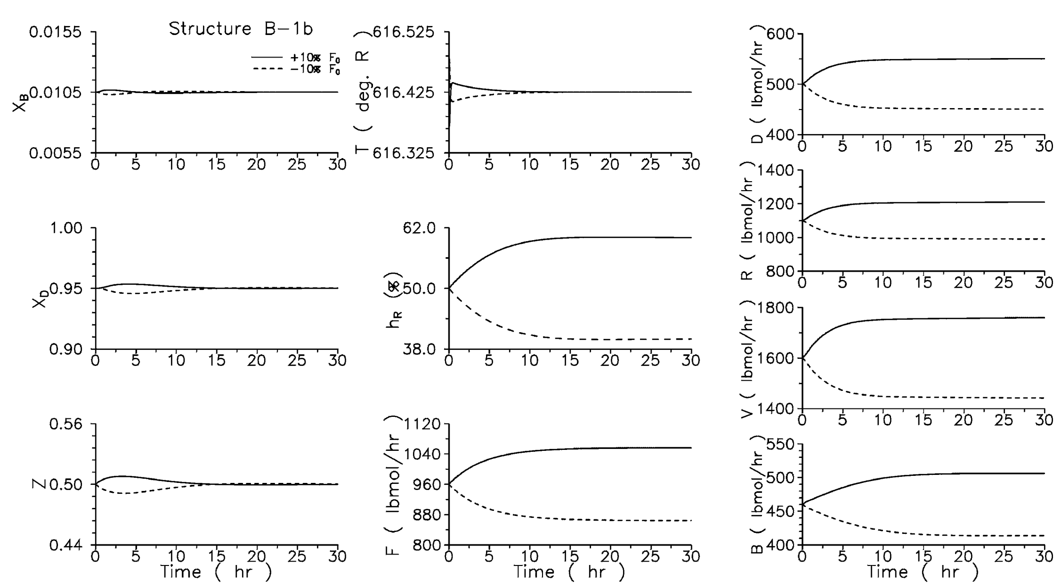

Fig. 19. Step responses of B-1b control structure for ±10% production rate changes.

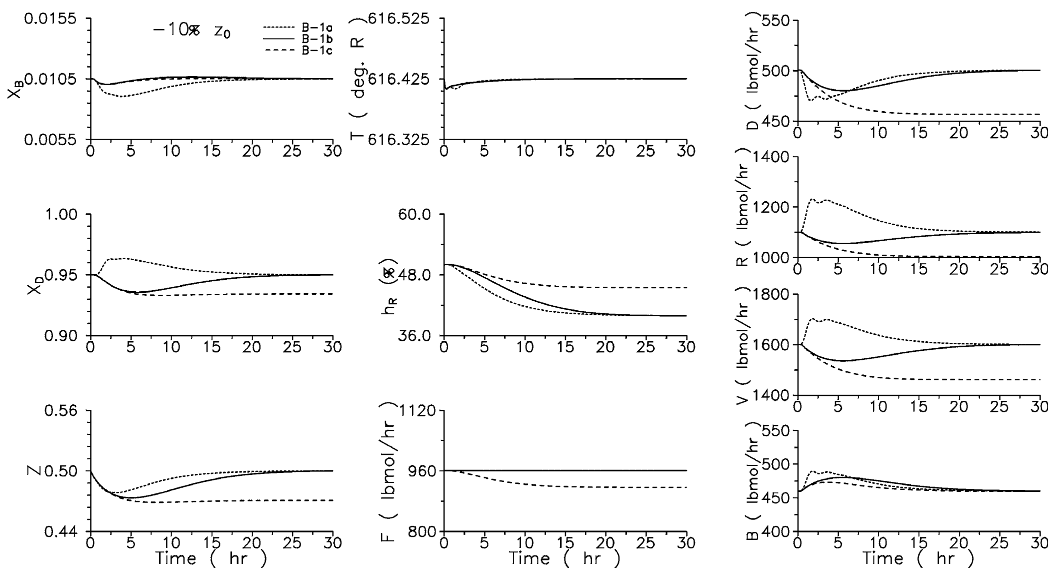

Fig. 20. Step responses of B-1a, B-1b, and B-1c control structures for a 10% decrease in fresh feed composition.

fixing the V_R/F ratio via the level control. Consider the B-1c control structure.

1) The fresh feed is flow controlled.
2) The reactor level is controlled using the reactor effluent flow rate (F) and a P-only level controller is used (i.e., allowing the reactor level to change as the production rate varies).
3) The reflux ratio (rR) is fixed.
4) The reflux drum level is maintained by changing the reflux flow and the base level is controlled by adjusting the bottoms flow.
5) The reactor temperature is controlled by the cooling water flow.
6) The bottoms composition (x_B) is controlled by changing the boilup ratio (BR).

The B-1c control structure consists of one composition loop and three level loops with one constant flow ratios. Table 3 compares the control loops for the class of B-1 structures.

6.2. Analyses

Under the premise of balanced structure, the next question then becomes: how do we set the proportional gain of the reactor level controller. Consider the material balances around the reactor with the assumption that we have perfect material balance for the column. The block diagram (Fig. 22) shows the relationship between the reactor holdup (V_R) and corresponding flow rates (F, F_0 and D). The process transfer function for the reactor holdup is simply an integrator ($G(s) = -1/s$) and a P-only controller is used ($K(s) = K_c$). Therefore, the closed-loop relationships are:

$$\frac{V_R}{F_0} = \frac{\dfrac{1+RR}{K_c}}{\dfrac{1+RR}{K_c}s + 1} \tag{24}$$

$$\frac{F}{F_0} = \frac{1+RR}{\dfrac{1+RR}{K_c}s + 1} \tag{25}$$

Divide Eq. (24) by Eq. (25), we have:

$$\left(\frac{V_R}{F}\right)_{(s)} = \frac{1}{K_c} \tag{26}$$

Since we would like to keep the residence time constant in the face of production rate change, the controller gain becomes:

$$K_c = \frac{1}{\tau_{res}} = \left(\frac{\bar{F}}{\bar{V}_R}\right) \tag{27}$$

In other words, the controller gain should be set as the inverse of the residence time. Using typical transmitter span and valve gain (e.g., Table 2), the dimensionless controller gain is simply *unity* (i.e., $K_c = 1$). In doing this, the residence remains constant for feed flow disturbance. This is a simple alternative for the reactor level control. Moreover, Eq. (25) indicates that the product flow rate following a first order dynamics with a time constant of $(1+RR)\tau_{res}$.

Fig. 16 shows the open-loop responses of the B-1c structure for a step feed flow change. The composition responses reveal that, in theory, we do not need *any* composition control for feed flow disturbances, because x_B, x_D and z return their steady-state values with the composition loop open as shown in Fig. 16. However, for the feed composition change, steady-state error in x_B

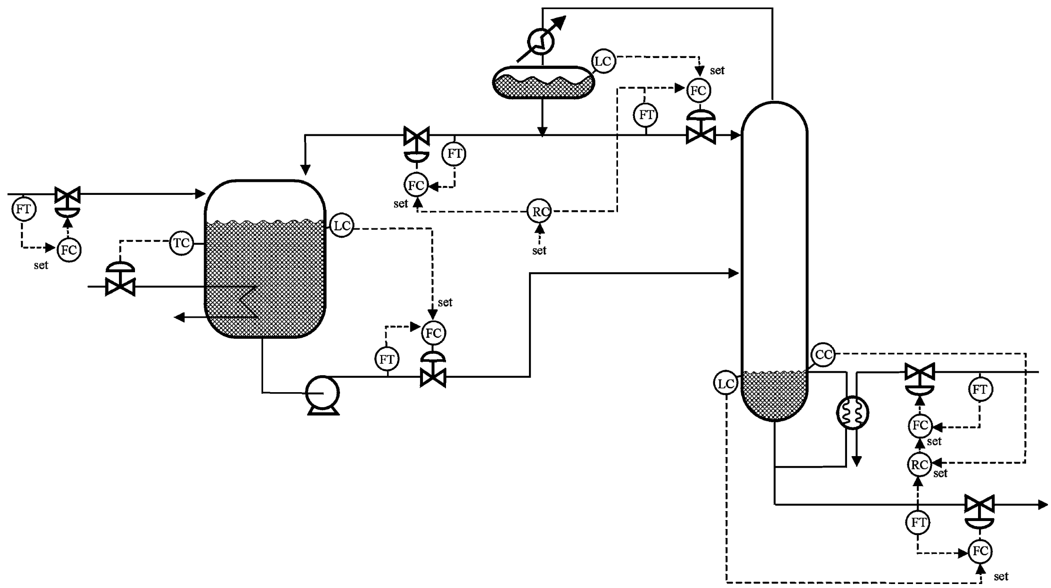

Fig. 21. B-1c control structure (control x_B, R/D, and V_R/F via P-control).

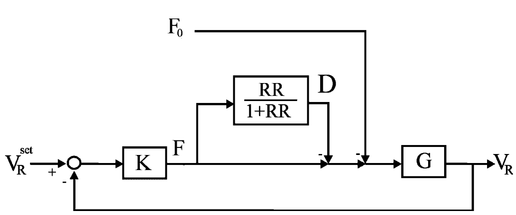

Fig. 22. Block diagram for the reactor holdup and corresponding flow rates.

occurs and, a composition controller is still needed to ensure the product quality for all possible disturbances. Following the same identification procedure of Section 5.2, the process and load transfer functions for the B-1c structure are given in Table 4. As indicated by open-loop load responses, we have a derivative (s) in (x_B/F_0)(s).

6.3. Results

Again, we can analyze the disturbance rejection capabilities in the frequency domain. The temperature and composition controllers are autotuned from relay feedback tests. Table 2 also gives the controller parameters for the B-1c structure. The closed-loop load transfer functions ($G_{L,CL}$) for feed flow and feed composition disturbances are shown in Figs. 17 and 18. As expected, a better load rejection in feed flow changes can be achieved using this structure (Fig. 17). For feed composition disturbance, the maximum peak heights are about the same for both B-1b and B-1c structures despite the B-1b structure showing better disturbance attenuation at low frequencies (as a result of two integrators in GK).

Time domain simulations show that the B-1c structure is practically the same as the B-1b structure. Fig. 23 shows good composition control can be achieved for $\pm$ 10% step changes in the fresh feed flow rates. Similar results are also observed for feed composition changes as shown in Fig. 20.

7. Conclusion

This paper considers the plantwide control structure design for improved disturbance rejection, in particular on the product composition. Based on steady-state disturbance sensitivity analysis, the full composition control structure is simplified to partial control using ratio schemes. More importantly, the disturbances sensitivity can be obtained from material balances. The results show that only one composition loop is sufficient to keep all three compositions near their set points. However, the B-1a control structure exhibits poor flow transition as production rate changes. In order to overcome the problems, two alternatives (B-1b and B-1c structures) are proposed. Only one composition and at most two flow ratios are controlled for the class of the B-1 control structures. A unique feature of the proposed B-1b control structure is that the reactor level is *not* controlled, because the reactor holdup has a steady-state effect and exhibits self-regulating behavior. This leaves us with only two level loops in the recycle plant. However, we need to design a feedforward controller to maintain the feed flow ratio. An alternative to keep a constant feed flow ratio (FR) is to use a P-only reactor level controller. By setting the controller gain to be the inverse of the reactor residence time, we are able to maintain a constant residence time and, subsequently,

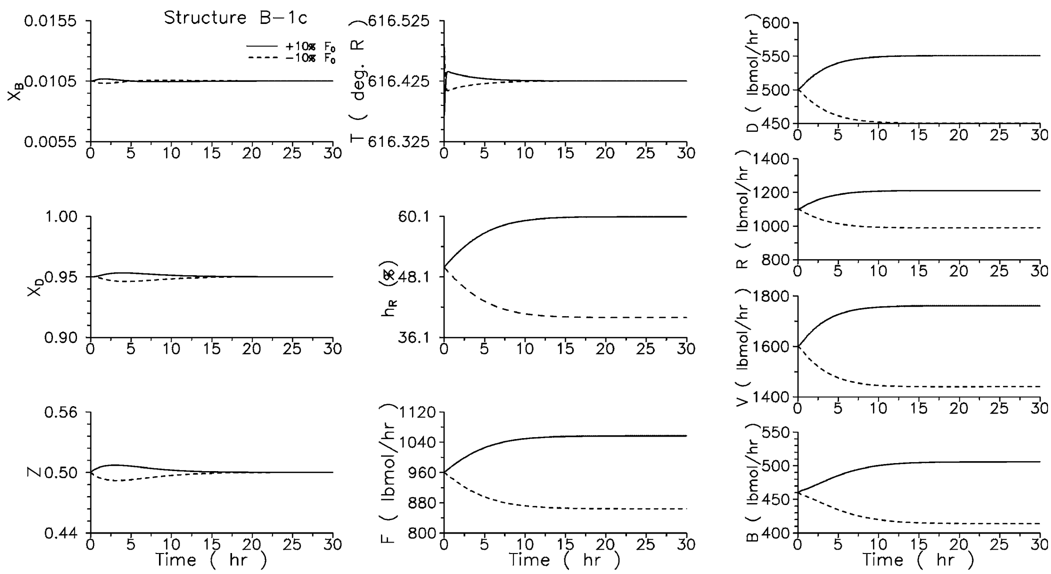

Fig. 23. Step responses of B-1c control structure for ±10% production rate changes.

the desired *FR*, in the face of feed flow disturbances (B-1c structure).

We have proposed a heuristic approach to control structure design for balanced control. It starts from 3 composition loops (B-3) to 2 composition loops plus 1 ratio (B-2), to 1 composition loop plus 2 ratios (B-1a), to 1 composition loop plus 1 ratio and floating reactor level (B-1b), and then to 1 composition loop plus 1 ratio and 1 P-only reactor level control (B-1c) (Table 3). The complexity of the instrumentation for the entire plant varies and judging on the dynamic performance we suggest B-1c (or possibly B-1b) as the candidate structure. The heuristic generated is: ‘use ratio (or similar concept, e.g., P-only level control or simply letting the level float) to eliminate composition loops’. Frequency and time domain analyses show that better product composition control can be achieved using B-1b and B-1c control structures for both feed flow and feed composition disturbances. Results also show that smoother flow transitions are also observed as the production rate changes. More importantly, this concept can be extended to different plantwide control problems in a straightforward manner.

Acknowledgements

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