Interaction of Process Design and Control

1. The 1st-Order Continuous Stirred Tank Reactors

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The task of the process design engineer focused on determining the flow sheet structure, parameter values, and steady-state operating conditions to meet the objectives, they are: minimize annual cost, maximize annual profit, etc. After a final design has been developed, it is passed over to the process control engineers. The task of control engineer then centered on establishing a control strategy to ensure stable dynamic performance and product quality requirements. It used to happen that the optimal design based on steady state and the controllability of a plant conflict to each other. It is better to consider the interaction between these two tasks and aims to build a process that has little higher capital and energy costs but provides more stable operation and achieves less variability in product quality.

Consider a one or more CSTRs in series for example. In this CSTR system,

1. a 1st order irreversible exothermic reaction takes place; $r_n = V_n k_n z_n$,
2. all reactors have the same volume and operate at the same specified temperatrure,
3. L/D = 2, T=140°F, $r = 0.5\,hr^{-1}$, $\Delta H = 30,000 Btu/lb-mole$, $F = 100\ lb-mole/hr$
4. Feed temperature=70oF, zo=1, MW=50 lb/lb-mole
5. Liquid density=50 lb/ft^3,
6. Inlet cooling water temperature=70°F, U=300 Btu/hr/°F/ft^2

The steady-state design procedure is :

1. Specify the conversion χ,
2. Calculate the concentration leaving the system, z_n,
3. Calculate the size of the reactors,
4. Calculate the Geometrical parameters of the reactors, and determine the capital cost.
5. Calculate the heat removal rate and the related jacket temperature, cooling water flow rate for each reactor.

The material and Energy balances around each of the reactor are given as follows:

$$\frac{dz_n}{dt} = \left(\frac{F}{V_n}\right) z_{n-1} - \left(\frac{F}{V_n}\right) z_n - z_n k_n$$

$$\frac{dT_n}{dt} = \left(\frac{F}{V_n}\right) T_{n-1} - \left(\frac{F}{V_n}\right) T_n - \frac{\lambda z_n}{MC_p} k_n - \frac{UA_{H,n}}{C_p MV_n}(T_n - T_{J,n})$$

$$\frac{dT_{J,n}}{dt} = \left(\frac{F_{J,n}}{V_{J,n}}\right)(T_{J,o} - T_{J,n}) + \frac{UA_{H,n}}{C_J \rho_J V_{J,n}}(T_n - T_{J,n})$$

At Steady state, we have:

$$0 = \left(\frac{F}{V_n}\right) z_{n-1} - \left(\frac{F}{V_n}\right) z_n - z_n k_n \qquad (1)$$

$$0 = \left(\frac{F}{V_n}\right) T_{n-1} - \left(\frac{F}{V_n}\right) T_n - \frac{\lambda z_n}{MC_p} k_n - \frac{UA_{H,n}}{C_p MV_n}(T_n - T_{J,n}) \qquad (2)$$

$$0 = \left(\frac{F_{J,n}}{V_{J,n}}\right)(T_{J,o} - T_{J,n}) + \frac{UA_{H,n}}{C_J \rho_J V_{J,n}}(T_n - T_{J,n}) \qquad (3)$$

Let, $Z_n = Z_o\,(1\text{-}x)$, where x is the conversion of the reaction.

For N=1, we have: $Z_1 = Z_o\,(1\text{-}x)$. From Eqn.(1), we found:

$$\frac{F}{V_1} z_o - \frac{F}{V_1} z_o (1-x) - z_o (1-x) k_1 = 0$$

So, we have:

$$V_1 = \frac{Fx}{(1-x)k_1}$$

Similarly, it can be shown that:

For N=2,

$$V_1 = V_2 = \frac{F(1-\sqrt{1-x})}{k\sqrt{1-x}}; \quad z_1 = \frac{z_o F}{F + V_1 k}; \quad z_2 = (1-x) z_o$$

and, N=3, we have:

$$V_1 = V_2 = V_3 = \frac{F[1-(1-x)^{1/3}]}{k(1-x)^{1/3}};$$

$$z_1 = \frac{Fz_o}{F + V_1 k_1}; \quad z_2 = \frac{Fz_1}{F + V_2 k_2}; \quad z_3 = z_o (1-x)$$

According to J.M.Douglas (Conceptual Design of Chemical Processes, 1988), the cost can be estimated as:

$$D_n = \left(\frac{2V_n}{\pi}\right)^{1/3}; \quad L_n = 2D_n; \text{ Cost} = 1916.9(D_n)^{1.066}(L_n)^{0.802}; \quad A = 2\pi(D_n)^2$$

Let: $Q_n = C_P MF(T_{n-1} - T_n) - \lambda z_n V_n k_n$

We start with the energy balance for the reactor:

$$\frac{UA}{C_P MV_n}(T_n - T_{J,n}) = \frac{F}{V_n}(T_{n-1} - T_n) - \frac{\lambda z_n k}{MC_P}$$

So,

$$T_n - T_{J,n} = \frac{1}{UA}\left[FMC_P(T_{n-1} - T_n) - \lambda z_n V_n k\right]$$

$$= \frac{1}{UA}\left[FMC_P(T_{n-1} - T_n) - \lambda (z_{n-1} - z_n)F\right]$$

$$= \frac{1}{UA}Q_n \quad \Rightarrow \quad T_{J,n} = T_n - \frac{1}{UA}Q_n$$

$$Q_1 = -\lambda(z_0 - z_1)F + C_P MF(T_1 - T_o)$$

$$\vdots$$

$$Q_n = -\lambda(z_{n-1} - z_n)F + C_P MF(T_n - T_{n-1})$$

And,

$$\frac{F_{J,n}}{V_{J,n}}(T_{J,n} - T_{J,o}) = \frac{UA}{C_J \rho_J V_{J,n}}(T_n - T_{J,n})$$

or,

$$F_{J,n} = \frac{UA}{C_J \rho_J (T_{J,n} - T_{J,o})}(T_n - T_{J,n}) = \frac{Q_n}{C_J \rho_J (T_{J,n} - T_{J,o})}$$

Thus, All the quantities such as: $V_n, z_n, Q_n, T_n, F_{J,N}$ can be calculated.

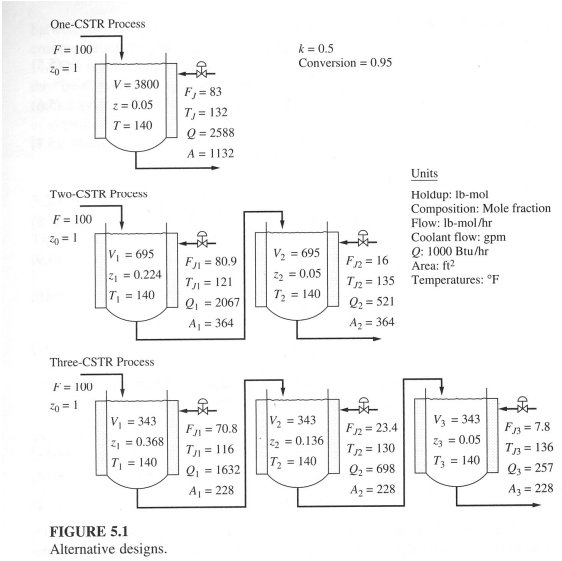


FIGURE 5.1
Alternative designs.

The capital costs of some of the alternative processes are summarized as follows:

Case 1: k=0.5 and 95% conversion

Cost of one-CSTR process =$427,300

Cost of two-reactor process = $296,600

Cost of three-CSTR process =$286,700

Case 2: k=0.5 and 99% conversion

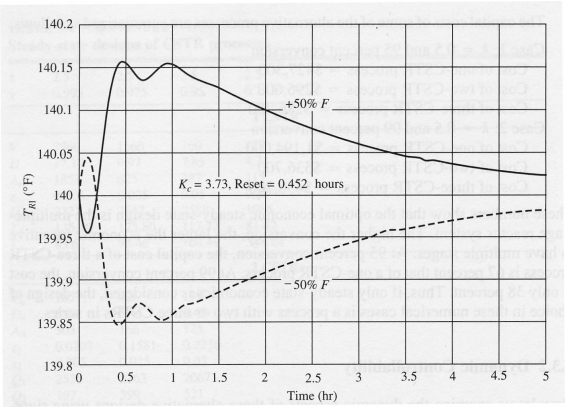
Cost of one-CSTR process =$1,194,000

Cost of two-reactor process = $536,700

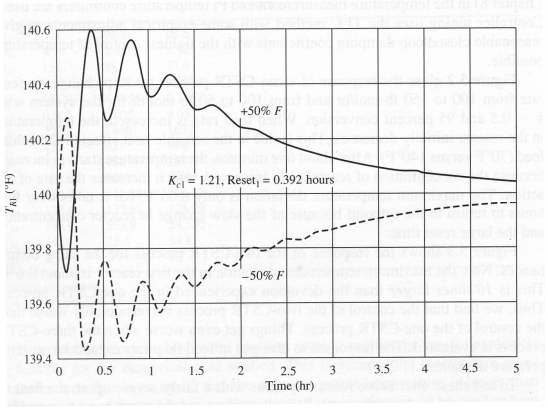
Cost of three-CSTR process =$458,200

The results show that an optimal design of the reactor system favors multistage reactors.

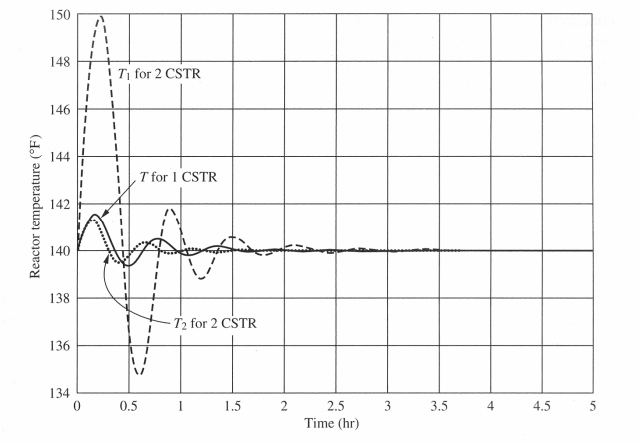
Then, we consider the dynamic controllability of these processes. In each of the process, PI controllers tuned by TLC method are used. The temperature measure has two one-minute first-order lags.



95% conversion, one-reactor system



Two reactor system



50% reaction heat increase

The results clearly demonstrate that the most economical process from a steady-state point of view is not the best from a dynamic point of view.

Controllability Incentives

Difficult ←---------- Control of reactor Temperature ←---------- Easy

| ←--------decreases---------- Reactor Holdup -------increase ---------→|

| ←--------increase ---------- Heat Removal Rate ------ decrease --------→|

| ←--------decrease ---------- Reactor Size --------increase ---------→|

Economics Incentives

High ←---------- no. of stages ----------→ Low

2. Control of heat integrated process

Introduction

Parallel process units are often encountered in chemical process systems for different considerations, e.g., parallel reactors from reactor network synthesis, parallel columns for heat integration. One notable example is the feed split configuration of heat-integrated distillation column (King, 1980; Chiang and Luyben, 1983; Andrecovich and Westerberg, 1985) where the feed is splitted into two streams and are fed to two columns which are heat-integrated. In doing this, 50% energy saving can be achieved.

Extensive literature on the design and control of heat-integrated distillation systems have been reported. Tyreus and Luyben (1976) examine the control issue of double-effect distillation and an auxiliary reboiler is suggested for improved control performance. Chiang and Luyben (1988) study the control for three different heat-integration configurations: feed-split, light-split forward (integration), and light-split reverse. They concluded that the light-split reverse is the most controllable scheme. Weitz and Lewin (1996) study the same system using the disturbance cost as a controllability measure and a similar conclusion is drawn. Wang and Lee (2002) explore nonlinear PI control for binary high-purity heat-integrated columns with light split/reverse configuration. Yang et al. (2000) use a simplified model derived from state space equations to evaluate disturbance propagation for double-effect column under feed-split configuration. Interaction between design and control for heat-integrated and/or thermally coupled distillation systems are studied by Rix and Gelbe (2000) and Bildea and Dimian (1999) using dynamic RGA as a controllability measure. Lin and Yu (2003) explore the interaction between design and control for heat-integrated columns. However, few of these work takes advantage of the parallel characteristic of the processes into account. That is, in control structure design, one should emphasize on the output of the entire system instead of the output of individual (parallel) unit. The objective of this work is to explore the design and control of parallel processes and it is illustrated using heat-integrated distillation columns with feed split (FS) configuration.

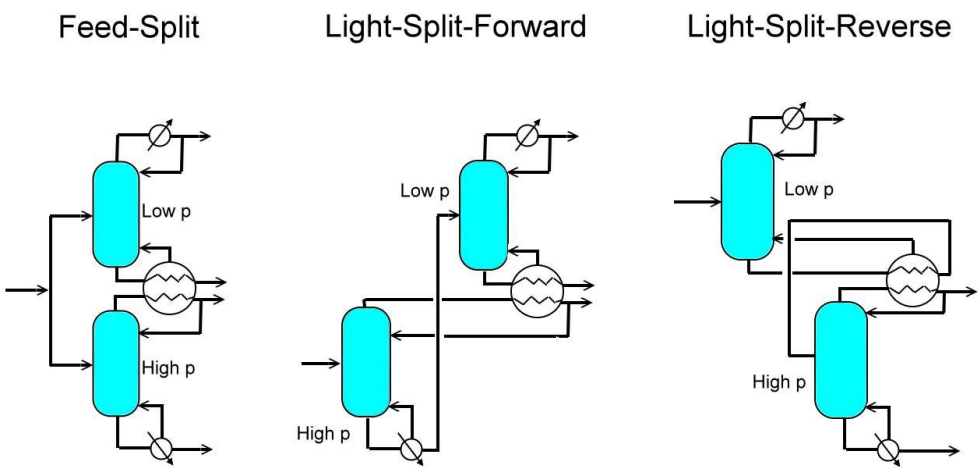


Figure 1 Three heat integrated systems

Process Configuration and Design Procedure

At the steady-state design, a systematic procedure is employed to find the number of trays and feed tray location. For the single column configuration, initially the reflux ratio is set to 1.2 times of the minimum reflux ratio (RR_{min}), then the number of trays and feed tray location are found by tray-by-tray calculation until the specification is reached, followed by refining the reflux ratio to meet the exact product specifications. For the heat-integrated systems, three configurations are considered: (1) feed split (FS), (2) light-split reserve (LSR), and light-split forward (LSF). Fig. 1 shows these three configurations where one column is pressurized and the high pressure column provides the heat to boilup the vapor in the low pressure column via condensation. Theses three configurations differ in the direction of material flow versus the direction of the heat-integration. Again, the "1.2 RR_{min}" criterion is used for the design of the heat-integrated column and 5% heat loss in the high pressure column is assume. That is heat transfer to the low pressure column via the heat exchange is limited to 95% of the heat of condensation in the high pressure column. 15 degrees of temperature driving force is assumed for heat transfer in all cases.

2.2 Steady-state Economics

Three systems are studied, they are: methanol-water, benzene-toluene, and isobutane-n-butane systems which correspond to high (α=2.45-7.58), medium (α=2.35-2.65), and low (α=1.29-1.30) relative volatilities, respectively. Table 1 compares the absolute energy consumption for these three chemical systems with

three different feed compositions (of light component). The results show that percent energy saving ranges from 32-41% for the feed-split configuration, from 3-36% for the light-split forward configuration, and from 14-43% for the light-split reverse configuration. The percent of energy saving clearly reveals that the feed split configuration consistently provides economical incentives over the conventional single column configuration. However, the FS configuration show four product streams and, in the context of process control, this implies that we have a system with four controlled variables, quite possibly a 4x4 multivariable system. A possible tradeoff between steady-state economics and dynamical controllability may result as compared to the 2x2 multivariable system in the conventional configuration.

Fig. 2 shows that the FS configuration is a typical parallel process where the products come from two parallel units and what we really care is the resultant composition after blending the product streams. That is, from a system perspective, we only need to control 2 product compositions, as opposed to the 4x4 control problem from the unit-wide perspective.

x_F	0.3	0.5	0.8
Methanol-Water			
FS	68%	64%	62%
LSF	75%	67%	64%
LSR	70%	61%	57%
Benzene-Toluene			
FS	66%	64%	61%
LSF	97%	81%	66%
LSR	86%	71%	59%
Isobutane-n-Butane			
FS	60%	59%	59%
LSF	80%	75%	67%
LSR	77%	70%	60%

	value		unit
Feed flow rate	10		*kmol/hr*
Feed composition	0.5		*m.f. of methanol*
	HP col	**LP col**	
Top composition	0.99	0.99	*m.f.*
Bottoms composition	0.01	0.01	*m.f.*
Column pressure	1	3.5	*atm*
Tray pressure drop	0.0085	0.0085	*atm*
Total no. of trays	36	57	
Feed location	21	35	
Reboiler duty		366166.3	*Btu/hr*
Approximated relative volatility	1.5~1.8	1.5~1.8	

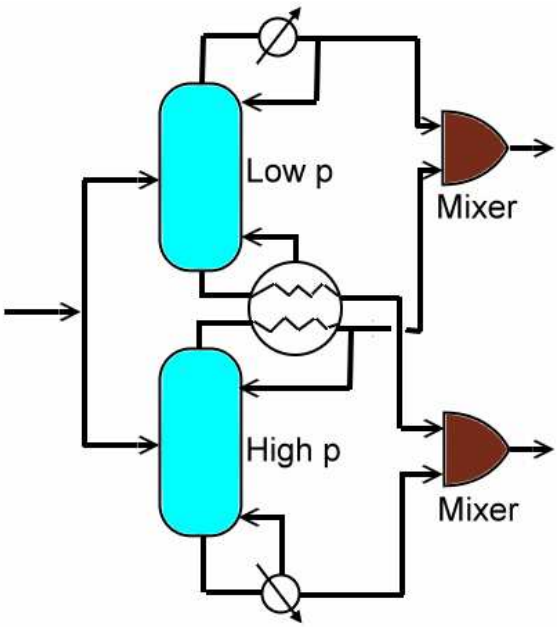


Figure 2 The parallel integrated system

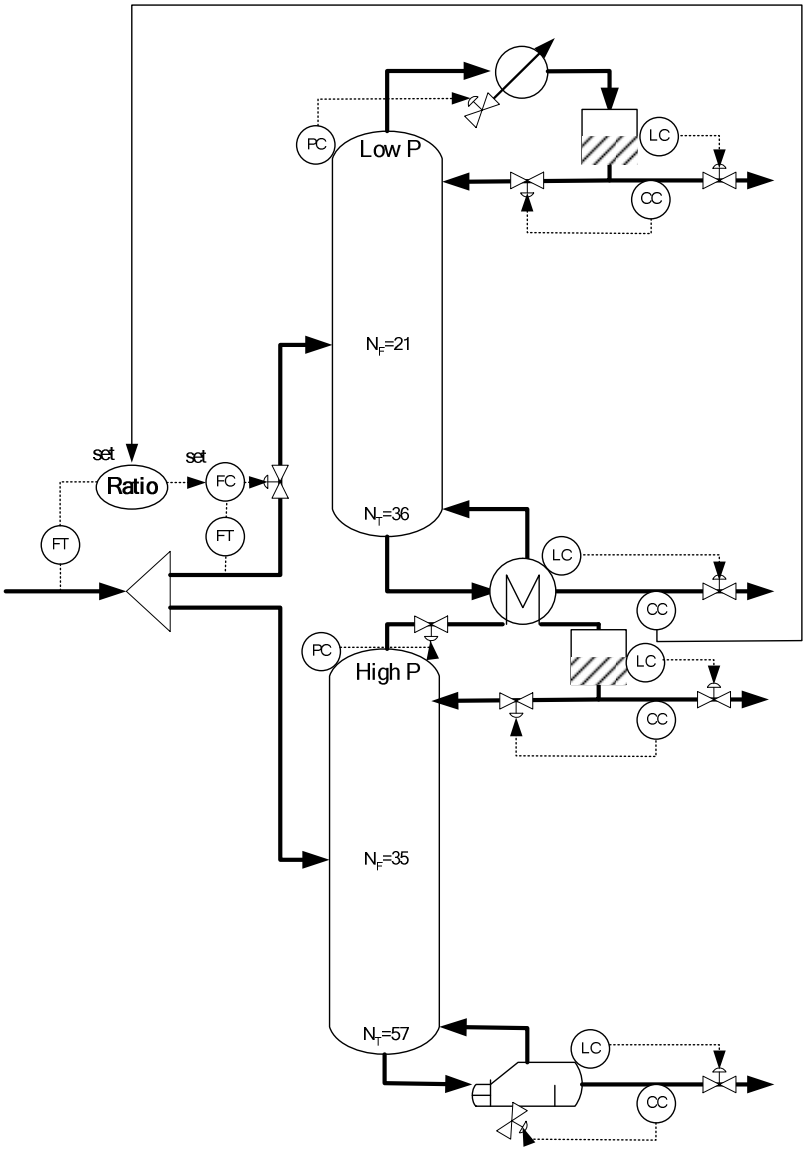


Fig. 3. Conventional control structure for the FS configuration with control structure S-1.

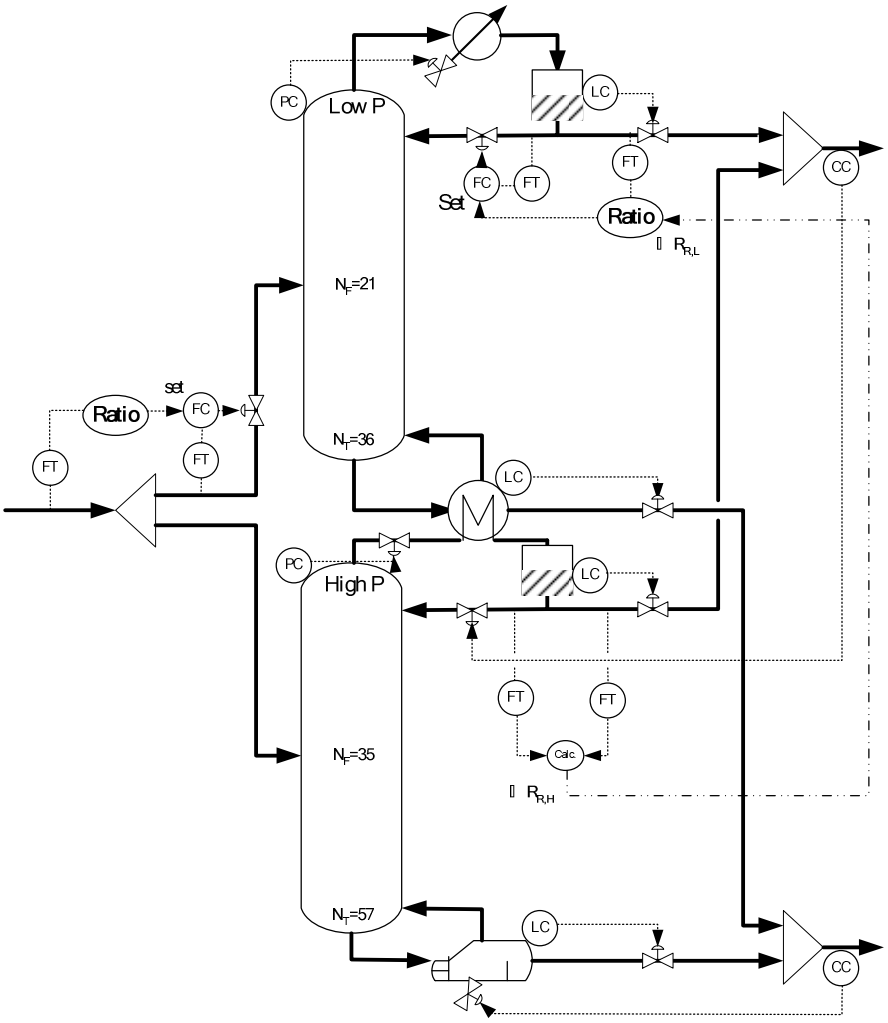


Fig. 4. Treating the FS heat-integrated column in parallel topology with control structure S-2

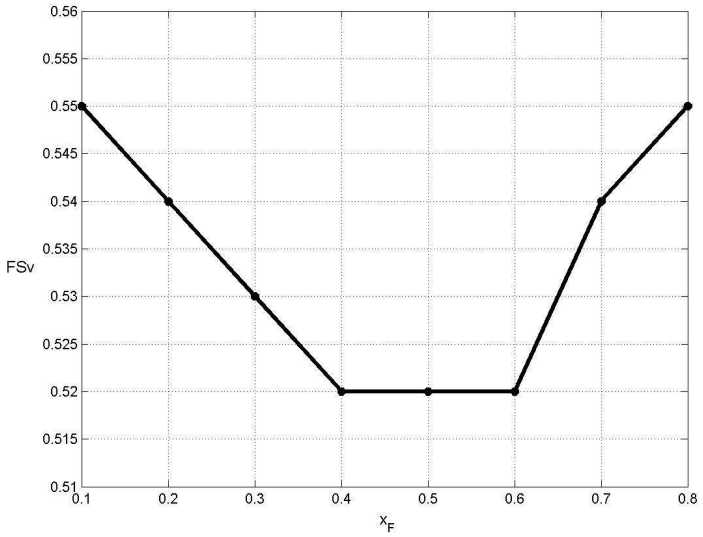


Fig. 5. The optimal feed ratio for different feed composition.

Controller Design

For the control structure S-1, the 4x4 process transfer function matrix is obtained from step tests. First order responses were assumed and the process transfer function matrix becomes:

$$\begin{bmatrix} x_{D,L} \\ x_{B,L} \\ x_{D,H} \\ x_{B,H} \end{bmatrix} = \begin{bmatrix} \frac{2.49e^{-3s}}{264.8s+1} & \frac{0.44e^{-3s}}{307.4s+1} & \frac{0.21e^{-3s}}{834.1s+1} & \frac{-3e^{-3s}}{278.4s+1} \\ \frac{2.59e^{-3s}}{284.9s+1} & \frac{0.56e^{-3s}}{190.8s+1} & \frac{0.16e^{-3s}}{585.9s+1} & \frac{-3.55e^{-3s}}{294.6s+1} \\ 0 & \frac{-0.56e^{-3s}}{493.8s+1} & \frac{2.61e^{-3s}}{450.5s+1} & \frac{-1.93e^{-3s}}{311.4s+1} \\ 0 & \frac{-1.2e^{-3s}}{319.5s+1} & \frac{3.27e^{-3s}}{322.2s+1} & \frac{-6.59e^{-3s}}{390.6s+1} \end{bmatrix} \begin{bmatrix} R_{F,L} \\ FS_V \\ R_{F,H} \\ Q_{B,H} \end{bmatrix} \quad (1)$$

A three minutes analyzer dead time is added to each transfer function for the composition measurement. Corresponding relative gain array is:

$$\Lambda = \begin{array}{c} \\ x_{D,L} \\ x_{B,L} \\ x_{D,H} \\ x_{B,H} \end{array} \begin{array}{c} \begin{array}{cccc} R_{F,L} & FS_V & R_{F,H} & Q_{B,H} \end{array} \\ \begin{bmatrix} 6.58 & -3.23 & -0.21 & -2.42 \\ -5.85 & 3.95 & 0.15 & 2.75 \\ 0 & -0.60 & 1.91 & -0.30 \\ 0 & 0.88 & -0.85 & 0.97 \end{bmatrix} \end{array} \quad (2)$$

Next, sequential design is taken to find the tuning constants of the decentralized

PID controllers (Huang et al., 2003). They are:

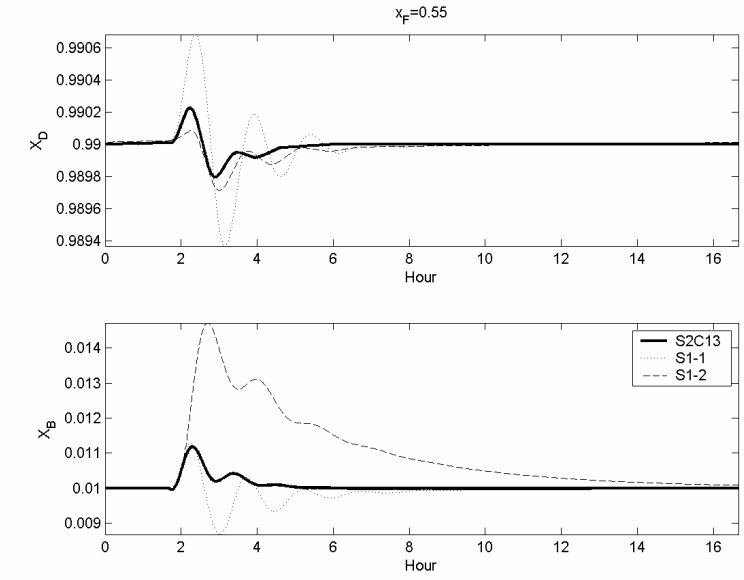
$$loop\ 1: K_c = 20.601 \quad \tau_I = 74.77 \quad \tau_D = 1.17$$
$$loop\ 2: K_c = 14.335 \quad \tau_I = 105.58 \quad \tau_D = 2.41$$
$$loop\ 3: K_c = 32.63 \quad \tau_I = 70.25 \quad \tau_D = 1.15$$
$$loop\ 4: K_c = -4.704 \quad \tau_I = 144.15 \quad \tau_D = 2.07$$

Because of its high dimensionality, a second set of tuning constants are obtained by reducing K_c to 60% and increasing reset time (τ_I) to 130% of their nominal values. For the control structure S-2, the 2x2 process transfer function matrix is also identified from step responses.

$$\begin{bmatrix} x_{D,mix} \\ x_{B,mix} \end{bmatrix} = \begin{bmatrix} \frac{3.06e^{-3s}}{347.4s+1} & \frac{-2.77e^{-3s}}{302.2s+1} \\ \frac{2.68e^{-3s}}{298s+1} & \frac{-5.42e^{-3s}}{366s+1} \end{bmatrix} \begin{bmatrix} R_{F,H} \\ Q_{B,H} \end{bmatrix} \tag{3}$$

This pairing gives a relative gain of 1.81. Again the sequential design approach is taken and PID settings become:

$$loop\ 1: K_c = 20.75 \quad \tau_I = 31.36 \quad \tau_D = 1.198$$
$$loop\ 2: K_c = -12.34 \quad \tau_I = 31.48 \quad \tau_D = 1.197$$



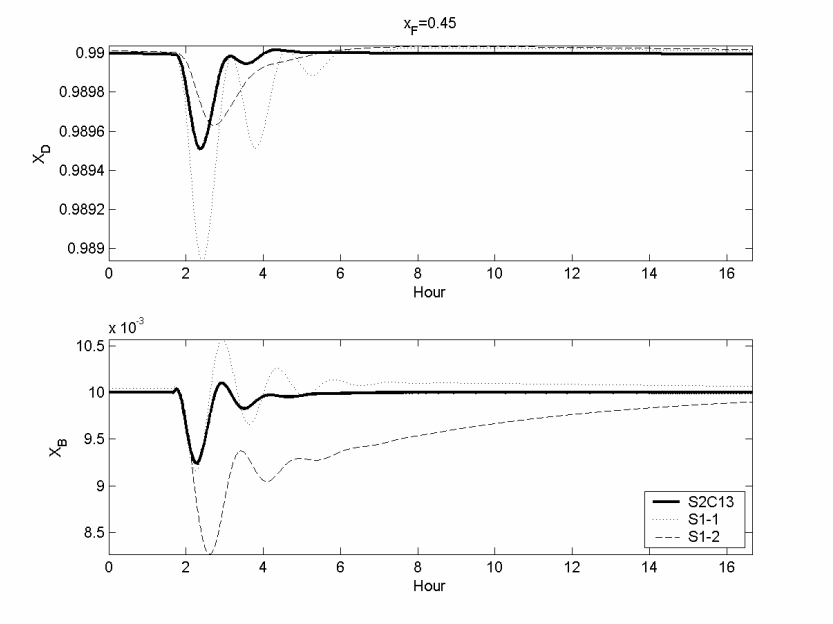
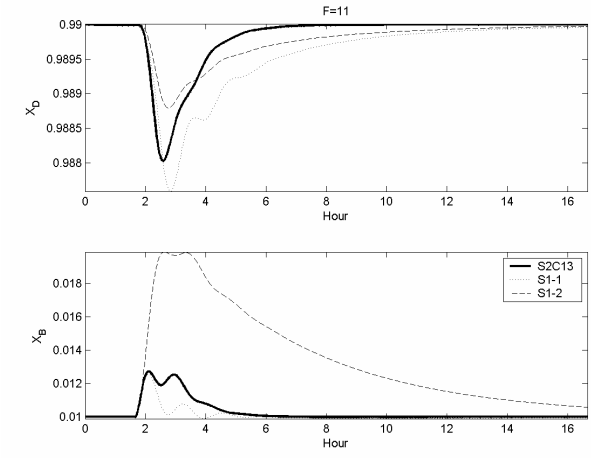


Fig.6 Responses for ±10% feed composition changes using control structures S-1 (tight tuning S1-1 and loose tuning S1-2)and S-2.



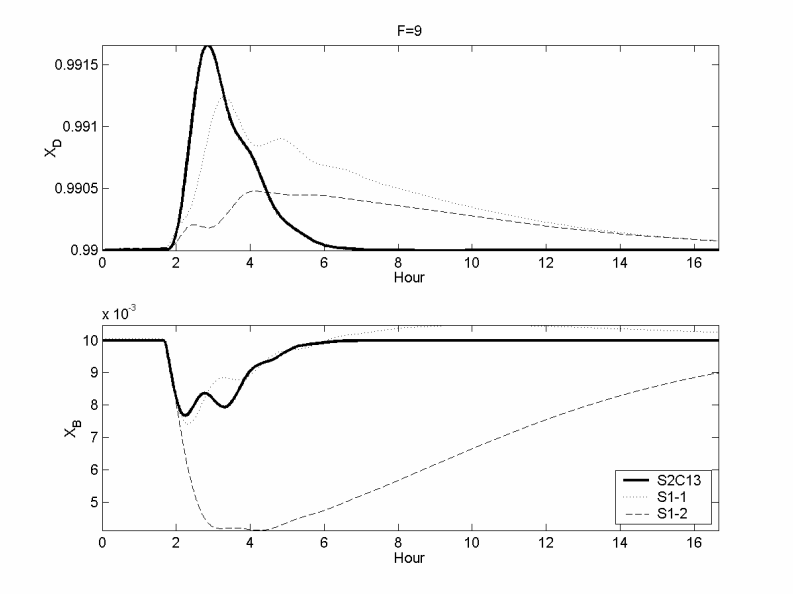


Fig. 7. Responses for ±10% feed flow rate changes using control structures S-1 (tight tuning S1-1 and loose tuning S1-2) and S-2.

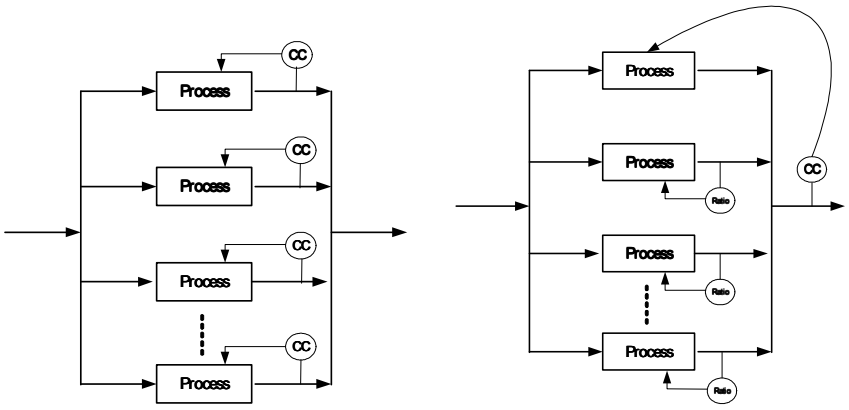


Fig. 8. Conventional control structure (A) versus treating the parallel unit as a system (B)

Control Performance and Discussion

Dynamic simulations were performed to compare performance of these two control structures. All simulations were carried out in ASPEN Dynamics. The results indicate that for ±10% feed composition changes, the simpler S-2 structure gives much better performance and the peak errors is consistently smaller than that of using control structure S-1 (Fig. 6). Note that two sets of tuning constants were evaluated under structure S-1: the tight tuning (S1-1) and loose tuning (S1-2). For ±10% feed flow rate composition changes, the closed-loop responses of S-2 are comparable to that of the control structure S-1 as shown in Fig. 7. The results presented here clearly show that improved control performance can be achieved using simpler control structure by taking the process topology into account. More importantly, for the heat-integrated columns, the improvement is obtained with virtually no loss in the economic objective (i.e., energy consumption).

The concept of treating the parallel units as a whole seems to offer an attractive alternative to control such processes. The advantages can be more evident if the number of units increases (Fig. 8). Still limitations are also observed for such a control strategy. An obvious one is that the ability to handle wide range of disturbances. Consider the feed split configuration with control structures S-1 and S-2. Based on dynamic simulations, the ranges of feed composition changes can be handled by S-1 and S-2 are $0.1 \leq x_F \leq 0.9$ and $0.2 \leq x_F \leq 0.8$, respectively. The reason is that the feed ratio is fixed for the structure S-2. A second potential problem is that it may become difficult to use the simple single temperature control for the structure S-2. That is composition control or some type of soft sensor should be used.

Remarks

Parallel processes are often encountered in process industries. In control system design, we can take advantage of this type of process topology. In this work, the control of parallel processes is illustrated with the heat-integrated distillation column example. The feed-split configuration is known to provide significant energy saving over the traditional single column configuration

and it provides close to 50% energy saving over the system without heat-integration. However, the energy integration results in a highly interacting multivariable system with higher dimensionality and less control degrees of freedom. However, the parallel nature of the system leads to a completely different thinking of the control objective (as opposed to the conventional practice): control the global product composition at the end of the production line instead of the quality of each individual unit. This greatly simplifies the design procedure and subsequently results in a much simpler control system. The feed-split heat-integrated distillation example clearly shows that improved control performance can be achieved by taking the process topology into account. More importantly, this is obtained with much simpler hardware requirement as well as engineering manpower. The benefit can be much more substantial when the number of parallel units increases.

3. Incorporation of dynamic controllability to steady-state design

One of most important problems in process design and process control is how to incorporate dynamic controllability quantitatively into conventional steady state design. There are different approaches:

1. Constraint-based methods:--- Take the optimal steady state design and determine how far away from the optimal point the plant must operate in order not to violate constraints during dynamic upsets.

2. Weighting factor methods:--- To form a multi-objective optimization problem in which some factor related to dynamic controllability is added to the traditional steady state economic factor. These two factors are suitably weighted, and the sum of the two is optimized. The dynamic controllability factor can be some of the goodness of control, the cost of the control effort, or the value of some controllability measures.

3. Capacity-based methods--- The capacity factor is defined as the fraction of time

that the plant is producing on-specific product. Thus, a system that has good capacity has a larger capacity factor.

4. Use of steady state sensitivity analysis---- The idea is to specify a control structure (fixed the variables that are held constant in the control scheme) and specify a disturbance. Then solve the nonlinear algebraic equations to determine the values of all variables at the new steady state condition. The structure that has most resilience in operation will be the one that has best controllability.

5. Use of RGA

6. Screen the infeasible structure by using Niederlinski's index.

7. References

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