Design and control for recycle plants with heat-integrated separators

Shih-Wen Lin^a, Cheng-Ching Yu^{b,*}

^aDepartment of Chemical Engineering, National Taiwan University of Science and Technology, Taipei 106 07, Taiwan

^bDepartment of Chemical Engineering, National Taiwan University, Taipei 106 17, Taiwan

Received 8 November 2002; received in revised form 29 August 2003; accepted 5 September 2003

Abstract

This work analyzes the tradeoff between steady-state economics and dynamic controllability for heat-integrated recycle plants. The process consists of one reactor, two distillation columns, and two recycle streams first studied by Tyreus and Luyben (Ind. Eng. Chem. Res. 32 (1993) 1154) and further explored by Cheng and Yu (A.I.Ch.E. J. 49 (2003) 682) and, in this work, the two distillation columns are heat integrated. The design problem differs from typical column sequencing and heat-integration design, because we can *design* the reactor composition. Optimal trajectories for heat-integrated recycle plants with direct and indirect sequences are analyzed as the reactor composition of C (z_C) varies. Provided with correct direction for heat integration, at any given z_C , the flowsheet is established for both sequences. It turns out the heat-integrated recycle plant with direct sequence is economically optimal throughout the entire range of z_C . For dynamic controllability, the reachable production range is identified as the recycle ratios (recycle flow rate/production rate) vary. Results show that the steady-state controllability deteriorates gradually as the degree of heat integration increases and, to the extreme, at the 50% energy saving line, we have lost one control degree of freedom. However, if the recycle plant is optimally designed ($z_C \approx 0.6$), acceptable turndown ratio is observed and little tradeoff between steady-state economics and dynamic operability may result. Finally, rigorous nonlinear simulations are used to test control performance of different process configurations (with and without heat integration). The results reveal that improved control can be achieved for well-designed heat-integrated recycle plants (compared to the plants without energy integration). More importantly, better performance is achieved with up to 40% energy saving and close to 20% saving in total annual cost.

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Keywords: Heat integration; Recycle process; Plantwide control; Design and control

1. Introduction

Last decade has seen significant progress in the design of plantwide control systems and most of the work addresses the issue of control structure design or the effects of material recycle on overall process dynamics. The timely book of Luyben et al. (1999) and the review of Larsson and Skogestad (2000) provide an updated summary.

On the other hand, we have seen extensive literature on the design and control of heat-integrated distillation systems. 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 conclude 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 same conclusion is drawn. Han and Park (1996) use nonlinear model-based control to eliminate interaction for double-effect columns and good performance can be achieved for high-purity specification. 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 simplified model derived from state space equation 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. An optimization approach is taken by Bansal et al. (2000) to investigate the interaction of design and control for double-effect

* Corresponding author. Tel.: +886-2-3365-1759; fax: +886-2-3362-3040.

E-mail address: ccyu@ntu.edu.tw (C.C. Yu).

distillation. Rev et al. (2001) provide a comprehensive study on the energy saving for ternary systems. Separation configurations, internal thermal coupling and external heat-integration are explored.

However, much less work has been done on the practically important process: heat-integrated recycle plants where both material and energy recycles exist simultaneously. This work analyzes the tradeoff between steady-state economics and dynamic controllability for heat-integrated recycle plants. The process consists of one reactor, two distillation columns, and two recycle streams first studied by Tyreus and Luyben (1993) and further explored by Cheng and Yu (2003) and, in this work, the two distillation columns are heat integrated.

2. Steady-state economics

2.1. Process configurations

The process studied is a ternary system with the following reaction: $A + B \rightarrow C$ (Tyreus and Luyben, 1993; Cheng and Yu, 2003). Two reactants A and B are fed to a CSTR which is operated isothermally. The reaction is second order and the rate can be expressed as

$$R = kV_R z_A z_B, \quad (1)$$

where R is the reaction rate, k is the rate constant, z_A and z_B are the mole fractions for reactants A and B, and V_R is the reactor holdup. The reactor effluent is assumed to be a saturated liquid and contains a ternary mixture of A, B, and C, because some A and B remain unreacted. Here, A is the light component (LK), B is the heavy component (HK), and the product C is an intermediate boiler (IK) and relative volatilities are: $\alpha_A = 4$, $\alpha_B = 1$, and $\alpha_C = 2$ at atmospheric pressure. Table 1 gives physical properties of the reaction/separation system. To separate the intermediate boiler (C) from the

Fig. 1. Process flowsheet and specifications for the recycle plant with direct separation sequence.

high and low boiling reactants (A and B), we need two distillation columns with two possible distillation sequences, direct and indirect sequences. Fig. 1 shows the process flowsheet with the direct sequence (D) where reactant A (LK) is recycled from the top of the first column back to the reactor and reactant B (HK) is recycled from the bottom of the second column back to the reactor. Product specifications are also given in Fig. 1.

Most of the operating cost of the recycle plant in Fig. 1 comes from the energy cost in distillation columns. It is common to reduce the energy cost by heat integration of these two columns. For the direct separation sequence, two configurations exist: direct sequence with forward heat-integration (DF) and direct sequence with backward heat-integration (DB) as shown in Fig. 2A. Similarly, we have two possible configurations for the indirect separation sequence: indirect sequence with forward heat-integration (IF) and indirect sequence with backward heat-integration (IB) (Fig. 2B). The energy saving can be evaluated based on the vapor rate. For systems with heat integration, the total vapor rate is simply:

$$V_{TOT} = V_1 + V_2, \quad (2)$$

where V_1 and V_2 are the vapor rates for the first and the second column, respectively, and V_{TOT} is the total vapor rate. For all four configurations in Fig. 2, the total energy requirement relates directly to

$$V_{TOT} = \max(V_1, V_2). \quad (3)$$

Therefore, percent of energy saving can be computed and the incentives for heat integration (versus increased complexity in control and operation) can be evaluated immediately (Chiang and Luyben, 1983). This is the typical situation in the design of heat-integrated distillation systems. However, in the design of recycle plants, we face a very different scenario and the reason is that the feed to the separation section (i.e., reactor composition) can be *designed*. The role heat integration plays in the design of the entire plant is not clear and possible tradeoffs between energy saving and operation have not been explored.

Table 1
Basic physical properties for the reaction and separation system

Molecular weight (MW)	$MW_A = 50$, $MW_B = 50$, $MW_C = 100$
Averaged density (ρ_{avg})	75 (lb _m /ft ³)
Heat of vaporization (ΔH)	50000/3 (Btu/lbmol)
Reaction	$A + B \rightarrow C$
Rate expression	$R = kV_R z_A z_B$ (lbmol/h)
Rate constant	$k = 1$ (h ⁻¹) for nominal case
Relative volatility	$\alpha_A/\alpha_C/\alpha_B = 4/2/1$ for low-pressure column $\alpha_A/\alpha_C/\alpha_B = 3.24/1.8/1$ for high-pressure column
Temperatures	Computed from Clausius–Clapeyron equation $\frac{1}{T} - \frac{1}{T_0} = \frac{R}{\Delta H} \ln \frac{\sum \alpha_i x_i}{\sum \alpha_i x_{0,i}}$ Assuming normal boiling point of A of 200°F and temperature driving force for heat integration is 30°F

Fig. 2. Heat-integrated recycle plant with: (A) direct separation sequence (forward and backward integration); and (B) indirect separation sequence (forward/backward integration).

2.2. Generation of process flowsheet and total annual cost

Before getting to the steady-state design, the following assumptions are made. Using the direct sequence as an example (Fig. 2A), the assumptions are

- (1) The process components have constant density.
- (2) The flow rate of the product stream D_2 is fixed at 100 lbmol/h.
- (3) The product specification is $x_{D2,C} = 0.98$.
- (4) There is no component A leaving the bottom of the second column ($x_{B2,A} = 0$). Therefore, the composition of the heavy recycle stream B_2 is specified to be $x_{B2,B} = 0.99$, and $x_{B2,C} = 0.01$.
- (5) There is no component B leaving the top of the first column ($x_{D1,B} = 0$). Therefore, the composition of the light recycle stream D_1 is specified to be $x_{D1,A} = 0.99$, and $x_{D1,C} = 0.01$.
- (6) The relative volatility of the high-pressure column is assumed to be 90% of the lower pressure one (i.e., $\alpha_{i,HP} = 0.9\alpha_{i,LP}$; Chiang and Luyben, 1983).

With given specifications, we can complete the steady-state design for any given reactor product composition (z_C) and reactant distribution with different direction of heat integration. The steady-state conditions of all streams in the ternary recycle system are calculated from balance equations (Cheng and Yu, 2003). The low-pressure column is assumed to be at atmospheric and the pressure for the high-pressure column can be computed from the

Clausius–Clapeyron equation

$$P_i^{\text{sat}} = P_{i,0}^{\text{sat}} \exp \left[\frac{-\Delta H_i}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right], \quad (4)$$

where P^{sat} is the vapor pressure, ΔH is the heat of vaporization, and R is the gas constant. The temperatures are inferred from the following expression (Glinos, 1984):

$$\frac{1}{T} - \frac{1}{T_0} = \frac{R}{\Delta H} \ln \frac{\sum \alpha_i x_i}{\sum \alpha_i x_{0,i}}, \quad (5)$$

where the subscript 0 stands for a reference temperature. In this work, we assume the normal boiling point for the light component (A) is 200°F and temperature driving force for heat transfer is 30°F. With this assumption, we can compute the temperature on each tray.

Next, standard column shortcut approach is taken for the heat-integrated columns. First, the Fenske equation is applied to find the minimum number of trays ($N_{T,\min}$) and total number of trays is set to twice of $N_{T,\min}$ and the feed tray is located with the Kirkbride equation. Next, provided with assumed physical properties, the column is sized, tray holdup is computed, and liquid hydraulic time constant is computed as shown in the appendix. The heat transfer areas for the reboiler and condenser are also computed from the vapor flow rates (see the appendix). The reactor is also sized assuming an aspect ratio of 2. From steady-state design, we can determine all the process flow rates and the equipment sizes. Before leaving the design section it should be emphasized that a standard column design procedure ($N_T = 2N_{T,\min}$) is adapted here for the design of heat-integrated columns. As pointed out by one of the reviewer that an additional

Fig. 3. Optimal TAC trajectories (the reactant distribution showing minimum TAC for a given z_C) for recycle plant with direct (solid) and indirect (dashed) sequence and the boundary (thick solid) giving the same TAC for both sequences.

energy saving can be achieved by varying the numbers of trays such that $V_{\text{supply}} = V_{\text{demand}}$ and this will be useful when the heat-integrated columns of the recycle plant are not designed at 50% energy saving point (i.e., $V_1 \neq V_2$).

In order to select the best steady-state design for direct or indirect sequence, we employ economic assessment to evaluate different designs. The capital cost and operation cost of the entire plant are estimated using the correlation given in Douglas (1988) and the operating cost (primarily energy cost) is also obtained from vapor boilup. Provided with column base temperature, corresponding steam costs can be computed (appendix). Assuming payback years of 3 years, the total annual cost (TAC) model can be expressed as

$$\text{TAC} = \frac{\text{capital cost}}{3} + \text{operating cost.} \quad (6)$$

The TAC can be used to discriminate different process designs.

Provided with design specifications and economic measure (TAC), optimization is performed next. Given a specific separation sequence, we have two design degrees of freedom for the recycle plant. One is the reactant distribution z_A/z_B and the other is the conversion (or reactor composition of C, z_C). The optimization is carried out sequentially. First, the optimal reactant distribution is located for different z_C . These optimum reactant distributions are denoted as the optimal TAC trajectory. Fig. 3 shows the optimal reactant distribution for the direct (D) as well as the indirect (I) separation sequences when z_C varies from 0 to 1 (Malone et al., 1985; Glinos and Malone, 1988). Next, the TACs along the optimal trajectories are compared for

Fig. 4. 50% energy saving line ($V_1 = V_2$) for given z_C with direct (left) and indirect (right) sequences.

different z_C 's and the optimal design for each sequence can be obtained. Finally, the results of two different separation sequences are compared and the true optimal design is thus obtained. The last step can be made easy by drawing a boundary (indicated by thick solid line) which defines where the indirect (left-hand side) sequence and the direct sequence (right-hand side) are favored. Therefore, the true optimal design may be obtained by inspection of the optimality for each sequence. Cheng and Yu (2003) give detailed derivation for this boundary. For the flowsheet without energy integration, the results indicate that, for both sequences, the optimal paths start from the corner of heavy reactant (B) when z_C is low ($z_C \rightarrow 0$) and, as the z_C increases, they converge toward the center line which means equally distributed reactants (i.e., $z_A = z_B$). This coincides with one's intuition, because, at low z_C , the operating cost of distillation columns dominates and excess heavy component reduces the vapor rate. At high z_C , the reactor cost dominates and a 50/50 distribution of reactants (i.e., $z_A/z_B = 1$) is preferred, because $z_A = z_B$ gives the smallest reactor volume when z_C is fixed. Fig. 3 also shows the optimal trajectories always lie in the composition space where the heavy reactant is greater or equal to the light reactant. A question naturally arises: Do these results also apply to heat-integrated systems?

2.3. Energy saving

2.3.1. Maximal percentage of energy saving and trajectory of minimal energy consumption

For heat-integrated distillation columns, the incentives for integration can best be seen in Fig. 4 where the line of equal vapor rate is drawn (i.e., $V_1 = V_2$). These lines (Fig. 4) correspond to 50% of energy saving. For the direct sequence (Fig. 4A), the 50% energy saving line lies on the region where the direct sequence is favored (e.g., thick solid line in Fig. 3), but, for the indirect sequence (Fig. 4B), the maximal possible energy saving line also lies in the region where the indirect sequence is *not* favored. That implies that, for the indirect sequence, percentage-wise, the 50% energy saving line may be attractive, but the *total* energy requirement may not be minimal.

Fig. 5 shows the optimal energy consumption path as z_C changes from zero to one. For the direct sequence, the

Fig. 5. Minimal energy consumption (minimum V_{TOT}) paths for a given z_C with heat-integrated recycle plant with direct and indirect sequences.

optimal path coincides with the 50% energy saving line (Figs. 4A and 5), but for the indirect sequence, the trajectory for the minimal energy usage is completely different from the 50% energy saving line (Fig. 4B). The reason is quite obvious, for the indirect sequence, for total energy requirement (e.g., $V_1 + V_2$) is less in the region where indirect sequence is favored (Fig. 3). This means that less substantial heat-integration is expected for the recycle plant with indirect separation sequence and a higher degree of heat-integration will occur for the direct sequence.

2.3.2. Direction of heat integration

Next, we explore the effects of the direction (e.g., forward or backward) of heat integration on the total annual cost. Two cases are considered: one is the case of $V_1 \neq V_2$, and the other is $V_1 = V_2$.

Let us use the direct sequence to illustrate the effect of heat-integration direction. First, consider the case of $V_1 < V_2$. From thermodynamics perspective, the forward heat-integration configuration (DF) should be avoided, because this will lead to a higher pressure in the high-pressure column (the pressure in the low-pressure column is 1 atm). However, the required vapor rate for DF is simply $V_{TOT} = V_{2,LP}$ (Eq. (3)). On the other hand, if the DB configuration is employed, we have a lower pressure in the high-pressure column, but the vapor rate becomes: $V_{TOT} = V_{2,HP}$. Note that relative volatility, generally, decreases with a pressure increase. Therefore, we expect $V_{2,HP} > V_{2,LP}$ and, thus a higher energy requirement with DB configuration. Unless, the difference in the steam pressure (from pressure and subsequently temperature difference) can offset this increase in the vapor rate, DF configuration is favored in this case for its lower energy consumption. Therefore, the general rule is: integrate from the column with a smaller vapor rate (V_{small}) to the column

Fig. 6. Total annual costs with different directions in heat integration for recycle plant with direct separation sequence with different reactant distribution when $z_C = 0.6$.

with a larger vapor rate (V_{large}). Fig. 6 shows the TAC for the direct sequence with different directions of heat integration. The results show the suggested integration direction, $V_{small} \rightarrow V_{large}$, gives lower TAC throughout the entire range of reactant distribution.

For the case of $V_1 = V_2$, either the forward integration or the backward integration will give the same energy consumption. The backward integration (DB) has a small advantage because of a lower pressure and, thus, lower steam temperature. However, the difference in TAC is less than 1% over the entire range of z_C .

2.3.3. Optimal TAC trajectory and corresponding process flowsheet

Fig. 7 show the optimal TAC trajectory for the direct sequence as z_C varies from 0 to 1. Unlike the case of non-integrated recycle plant (e.g., Fig. 3), it follows the 50% energy saving line at low z_C ($z_C < 0.5$) and converges toward the center line ($z_A/z_B = 1$) at high product composition ($z_C \rightarrow 1$). The reason for that is, at low z_C , the operating cost of distillation columns dominates and high degree of heat integration reduces the vapor rate by half. At high z_C , the reactor cost dominates and a 50/50 distribution of reactants is favored. As for the direction of heat integration, at low z_C , either backward or forward heat integration can be chosen, but at high z_C , forward direction is preferred (DF) as shown in Fig. 7.

A very different trajectory is observed for the indirect sequence as shown in Fig. 8. It looks quite similar to that of non-integrated system (cf. Fig. 3), but at a lower TAC

Fig. 7. Optimal TAC trajectory (x) and corresponding direction(s) for heat integration for recycle plant with direct separation sequence (minimal energy consumption trajectory (circle) also shown).

Fig. 8. Optimal TAC trajectory and corresponding direction for heat integration for recycle plant with indirect separation sequence.

as the result of heat integration. But the optimal trajectory is far away from the 50% energy saving line, and, therefore, a lesser degree of heat integration is encountered. The optimal path starts from the corner of heavy reactant (B) and converges toward the center line for the same reason as explained earlier. Since this is the region where $V_1 > V_2$ (Fig. 4B), backward integration (IB) is the optimal one throughout the entire range of z_C .

Fig. 9A compares the TACs for three different cases: without heat integration, direct sequence with heat integration, and indirect sequence with heat integration. As expected, the heat-integrated plant with direct sequence gives the lowest TAC. Fig. 9B shows the percent saving on TAC. For the direct sequence, it ranges from 5% to 20% and for the indirect sequence it is within 12%. At true optima ($z_C \approx 0.6$), a further 18% saving in TAC

Fig. 9. Optimal TACs for non-heat-integrated plant and heat-integrated recycle plants with direct and indirect sequences (A); and percent TAC saving for heat-integrated plants (B).

is expected for the direct sequence with forward heat integration.

3. Operability and control

3.1. Operability

Any 10–20% reduction in TAC certainly provides incentive for energy integration for the recycle system. The next question then becomes: Are these plants operable? In this work steady-state operability measure is employed. Following the approach originally proposed by Subramanian and Georgakis (2001) and further extended by Cheng and Yu (2003), we use the recycle ratio (recycle flow rate/product flow rate, e.g., RR_i) to evaluate the production rate handling

Fig. 10. Available input spaces (spanned by RR_1 and RR_2) and corresponding reachable output space (turndown ratio) for non-heat-integrated (A); heat-integrated direct sequence (B); and heat-integrated indirect sequence (C).

capability of the recycle plant. First, we let the recycle ratios to be halved and doubled to explore the reachable production rate. Fig. 10A shows the achievable production rates for the non-integrated system under indirect sequence. Certainly, the input space is the entire square defined by RR_1 and RR_2 , because they are two independent variables and we have two degrees of freedom. For the direct sequence with forward heat integration (DF), an auxiliary reboiler is installed to provide necessary heat input to the low-pressure column (e.g., Fig. 7) for the case of $V_1 \neq V_2$. It is reasonably assumed that the auxiliary reboiler can provide up to twice of its nominal steady-state heat input. Therefore, the input

space is a subset of the square as the result of heat integration as shown in Fig. 10B. Fig. 10B also shows that at low z_C (e.g., $z_C < 0.5$), the distillation system is design along the 50% energy saving line ($V_1 = V_2$). This is a complete heat-integrated system and no auxiliary reboiler is required, and we are left with only one degree of freedom (Fig. 7). Thus, the input space becomes a line in the two-dimensional space as shown in Fig. 10B. Therefore, some degree of freedom is lost as the result of heat integration and its severity depends on the degree of heat integration (it becomes most severe at the 50% energy saving line). The input space for the indirect sequence is shown in Fig. 10C and the input almost spans the entire square because the optimal TAC path is far away from the 50% energy saving line (Fig. 4B).

The available input space does indicate the tradeoff between energy saving and operability (Fig. 10) as a result of loss of degree of freedom. As expected, the non-integrated system gives the largest turndown ratio over the entire range of z_C along the optimal path (Fig. 10A) and the indirect sequence with backward integration (IB) shows a little smaller but also good turndown ratio. However, for the most economical direct sequence with backward/forward heat integration results in very small reachable production range at low z_C (e.g., $z_C < 0.2$) and becomes acceptable at higher z_C (e.g., $z_C > 0.5$) and, fortunately, the optimal TAC trajectory does *not* coincide with the 50% energy saving line.

Therefore, tradeoff between steady-state economic (i.e., lower TAC via heat integration) and operability is encountered for recycle plant at low z_C (i.e., if the process has to be operated at low z_C). But at true economic optima ($z_C \approx 0.6$), all three configurations give acceptable turndown ratios. Table 2 show the operating conditions at true optima for all three configurations (DF, IB, and D, i.e., direct sequence without heat integration).

3.2. Control

3.2.1. Control structure

As pointed out by Cheng and Yu (2003), no single control structure works well over the entire composition space. The principle is to determine the variable handling in the production rate variation. For example, when the reactor composition is used to accommodate production change, we should always let the smaller reactant composition float. In turns of recycle ratio or recycle flow rate, this implies that we should let the smaller flow or flow ratio float by fixing the larger one.

From optimal operating condition for the DF configuration has the following reactor composition $z_A = 0.22$, $z_B = 0.18$, and $z_C = 0.60$. This means we should fix the recycle ratio of the first column (recycling component A). In order to ensure expected amount of A recycle back to the reactor, the distillate composition of A in the first column is control as shown in Fig. 11. Furthermore, ratio schemes are employed throughout to provide better throughput handling capability

(e.g., a balanced scheme of Wu and Yu, 1996). Once the basic strategy is set, the 11 control degrees of freedom are arranged as follows (Fig. 11):

1. The production rate is set by the fresh feed of B (F_{0B}).
2. The reactor holdup is held constant by controlling reactor effluent flow rate (F).
3. The recycle ratio of the first column ($RR_1 = D_1/D_2$) is fixed.
4. The top composition of the first column ($x_{D1,A}$) is controlled by changing reflux ratio (R_1/D_1).
5. The top level of the first column is controlled by manipulating the fresh feed of reactant A (F_{0A}).
6. The boilup ratio of the first column (V_1/B_1) is fixed.
7. The bottom level of the first column is controlled by changing the bottom flow rate (B_1).
8. The product composition ($x_{D2,C}$) is held by manipulating the reflux ratio of the second column (R_2/D_2).
9. The boilup ratio of the second column (V_2/B_2) is fixed.
10. The top level of the second column is controlled by manipulating the production rate (D_2).
11. The bottom level of the second column is controlled by changing the bottom flow rate (B_2).

The optimal reactant composition (Table 2) for the IB is: $z_A = 0.14$, $z_B = 0.24$, and $z_C = 0.62$. Therefore, the recycle flow (or recycle ratio) related to component B should be fixed. With this basic strategy, a control structure can be constructed and it is almost the mirror image of the DF configuration as shown in Fig. 12. Note that the true optima for both heat-integrated systems are located at region where $V_1 \neq V_2$ and auxiliary reboilers are required to provide additional heat to meet the total energy requirement. Therefore, similar to the system without heat-integration, both configurations have 11 control degrees of freedom. For the purpose of comparison, the optimal design for the recycle plant *without* heat integration is also shown in Table 2. This corresponds to the direct sequence (D) and the control structure is exactly the same as Fig. 11 except that the separators are not heat integrated.

3.2.2. Controller design

Nonlinear simulation is carried out to test the dynamics and control of the recycle plant. The column model is similar to the ideal distillation model of Luyben (1990) except this is a multicomponent version. It consists of NC ordinary differential equations (ODEs) for the reactor, NC($NT_i + 2$) for the i th column. It was programmed in FORTRAN which is available upon request. For the purpose of control, 4 min of analyzer dead time is assumed for composition measurement. Let us use the direct sequence with forward integration (DF) in Fig. 11 to illustrate the controller design. The process consists of two composition loops, five level loops, and four flow (or ratio) loops. Typically, flow controller can be set directly and, in this work, perfect flow

Table 2

Optimal designs (minimum TAC) for direct sequence with forward integration (DF), indirect sequence with backward integration (IB), direct sequence without heat integration (D)

Flowsheet	DF	IB	D (WO)
1. CSTR			
Fresh feed of A (lb mol/h)	99	99	99
Fresh composition of A (mole fraction)	1	1	1
Fresh feed of B (lb mol/h)	99	99	99
Fresh composition of B (mole fraction)	1	1	1
Reactor holdup (V_R) (lb mol)	2475	2917	3200
Reactor effluent (F) (lb mol/h)	164.4	159.0	151.6
Reactor composition of A (z_A) (mole fraction)	0.22	0.14	0.16
Reactor composition of B (z_B) (mole fraction)	0.18	0.24	0.19
2. Distillation 1			
Distillate flow rate (lb mol/h)	35.53	121.5	23.38
Distillate temperature ($^{\circ}\text{F}$)	310.2	228.6	200.2
Composition of A in distillate (mole fraction)	0.99	0.183	0.99
Composition of B in distillate (mole fraction)	~ 0	0.008	~ 0
Composition of C in distillate (mole fraction)	0.01	0.809	0.01
Bottom flow rate (lb mol/h)	128.9	37.54	128.1
Bottom temperature ($^{\circ}\text{F}$)	361.8	280.2	244.2
Composition of A in bottom (mole fraction)	0.008	~ 0	0.008
Composition of B in bottom (mole fraction)	0.229	0.99	0.225
Composition of C in bottom (mole fraction)	0.763	0.01	0.767
Relative volatility ($\alpha_A/\alpha_C/\alpha_B$)	3.24/1.8/1	4/2/1	4/2/1
No. of trays	32	27	32
Feed tray	15	17	12
Vapor flow rate (lb mol/h)	243.4	293.3	179.9
3. Distillation 2			
Distillate flow rate (lb mol/h)	100	21.48	100
Distillate temperature ($^{\circ}\text{F}$)	238.7	310.2	237.8
Composition of A in distillate (mole fraction)	0.01	0.99	0.01
Composition of B in distillate (mole fraction)	0.01	~ 0	0.01
Composition of C in distillate (mole fraction)	0.98	0.01	0.98
Bottom flow rate (lb mol/h)	28.882	100	28.078
Bottom temperature ($^{\circ}\text{F}$)	280.2	353.5	280.2
Composition of A in bottom (mole fraction)	~ 0	0.01	~ 0
Composition of B in bottom (mole fraction)	0.99	0.01	0.99
Composition of C in bottom (mole fraction)	0.01	0.98	0.01
Relative volatility ($\alpha_A/\alpha_C/\alpha_B$)	4/2/1	3.24/1.8/1	4/2/1
No. of trays	27	32	27
Feed tray	18	13	19
Vapor flow rate (lb mol/h)	258.6	198.5	256.8
4. Cost			
Reactor cost (\$)	3.11E+05	3.43E+05	3.79E+05
Column cost (\$)	3.29E+05	3.67E+05	3.65E+05
Heat exchanger cost (\$)	6.43E+05	6.77E+05	7.84E+05
Operating cost (\$)	1.38E+05	1.48E+05	1.85E+05
Pay-back years	3	3	3
TAC (\$)	5.65E+05	6.11E+05	6.95E+05

control is assumed. In the five level loops, four of them are column reboiler or reflux drum holdups and one is the reactor holdup. Perfect level control is assumed for the column inventory and the reactor level PI controller is tuned by setting the closed-loop time constant 1/10th of the residence

time with a damping coefficient of 0.707 and this only requires steady-state operating data. So, in practice, only the two composition loops require plant testing and identification. Relay feedback test (Yu, 1999) is carried out on this multivariable system (Fig. 13) and it takes

Fig. 11. Control structure for DF configuration.

Fig. 12. Control structure for IB configuration.

Fig. 13. Relay feedback tests of composition loops for DF configuration.

approximately 4.5 h to complete the first round as shown in Fig. 13. Once the ultimate gain (K_u) and ultimate period (P_u) becomes available, the PI controller parameters, controller gain K_c and reset time τ_I , are obtained using Tyreus and Luyben tuning rule ($K_c = K_u/3$ and $\tau_I = 2P_u$). The same controller design procedure is applied to all three configurations.

3.2.3. Production rate changes

Before getting into the details of simulation results, it should be emphasized that these optimal designs (DF, IB, and D) correspond to different steady states (Table 2). For 20% production rate changes, simulation results show that the DF configuration gives the best performance and the product composition returns to set point in 8 h ($x_{D2,C}$ in Fig. 14A) as opposed to 16 h for the IB configuration ($x_{B2,C}$ in Fig. 14B) and for configuration without heat

Fig. 14. Closed-loop responses for +20% throughput changes with: (A) DF configuration; (B) IB configuration; and (C) direct sequence without heat integration (D).

Fig. 14. continued.

integration (D) ($x_{D2,C}$ in Fig. 14C). Nonlinear responses were observed as one compares the positive and negative changes. For production rate increase, most of the variables are held at the vicinity of nominal steady state. However, for a production decrease, the recycle stream with composition uncontrolled showing significant deviation from nominal values ($x_{B2,B}$ in Fig. 14A, $x_{D2,B}$ in Fig. 14B, and $x_{B2,B}$ in Fig. 14C). These responses indicate that some of the product C is recycled back to the reactor to make the term $kz_A z_B$ (rxn in Fig. 14) less than the nominal value.

3.2.4. Feed composition variations

At nominal cases, the fresh feeds are assumed to be pure A and B (100 mol%). Fig. 15 shows the responses when the fresh feed of A (F_{0A}) contains some impurity C and z_{0A} becomes 92% and 89%, respectively. Results shown that, for DF and IB configurations, product compositions ($x_{D2,C}$ in Fig. 15A and $x_{B2,C}$ in Fig. 15B) return to nominal values and most of the variables settle down in 100–200 h as shown in Fig. 15A and B. However, for the direct sequence without heat integration (D) with a –11% composition change, the control system fails to maintain product purity and some of the internal flows simply take off as shown in Fig. 15C.

Similarly, feed composition variations of fresh feed B (z_{0B}) are investigated and C is assumed to be the impu-

urity. Fig. 16A shows, for the DF configuration, the product composition $x_{D2,C}$ returns to the set point in less than 100 h. Oscillatory responses were observed for –11% feed composition disturbance, but the magnitude of deviation is reasonably small (e.g., $\Delta x_{D2,C} < 0.001$). For the IB configuration, good control can be achieved for –8% feed composition change. However, for –11% feed composition disturbance, the system becomes unstable as shown in Fig. 16B and the potential instability cannot be observed qualitatively until 700 h (almost 30 days) after the step load change. For the direct sequence without heat integration (D configuration), smooth load responses can be achieved for –8% feed composition change (Fig. 16C). However, for –11% feed composition disturbance, a limit cycle is observed and all process variables show sustained oscillation. The reason for the limit cycle is explained as follows. First, a significant decrease in the total amount of B leads to the stoichiometric imbalance and excess amount of A goes over to the second column. The composition loop tries to re-establish product composition by increasing reflux flow (R_2 , $t = 50$ –80 in Fig. 16C), this results in increased vapor boilup and base flow (V_2 and B_2 , $t = 50$ –80) and, subsequently, excess product C is recycled back to the reactor. An increase in z_C slows down and reaction rate and decrease the amount of A excess and this eventually leads to a smaller internal traffic in the second column and a decreased amount of recycled product C (B_2 , $t = 80$ –120). But again, the problem of A excess

Fig. 15. Closed-loop responses for -8% and -11% feed composition (z_{0A}) changes with: (A) DF configuration; (B) IB configuration; and (C) direct sequence without heat integration (D).

reappears. The scenario continues and a limit cycle results. In summary, the tolerable composition variation is around 10% and, again, the DF configuration gives better distur-

bance rejection capability. More importantly, the improved performance is obtained using heat-integrated system with a 20% lesser TAC.

Fig. 15. continued.

4. Conclusion

This work analyzes the tradeoff between steady-state economics and dynamic control for heat-integrated recycle plants. Optimal TAC trajectories for heat-integrated recycle plants with direct and indirect sequences are derived as z_C varies. The results indicate that, for the direct sequence, the trajectory follows the 50% energy saving line at low z_C and converges to the line where the reactants are equally distributed at high z_C . For the indirect sequence, the trajectory locates far away from the 50% energy saving line which also indicates a lesser degree of heat integration is expected. Provided with correct direction for heat integration, the flowsheet is established for both sequences. It turns out the heat-integrated recycle plant with direct sequence is economically optimal and backward integration (DB) is preferred at low z_C while the forward integration (DF) should be used for $z_C > 0.5$. For steady-state controllability, the reachable production range is identified as the recycle ratios vary. From the available input space, it is clear that controllability deteriorates gradually as the degree of heat integration increases and, at the 50% energy saving line, one control degree of freedom is lost. However, if the recycle plant is optimally designed ($z_C \approx 0.6$),

acceptable turndown ratio is observed and little tradeoff between steady-state economics and dynamic operability may result. Finally, rigorous nonlinear simulations are used to test control performance of different process configurations (with and without heat integration). The results reveal that improved control can be achieved for well-designed heat-integrated recycle plants (compared to the plants without energy integration) with up to 40% energy saving and close to 20% saving in total annual cost.

Notation

B_i	bottom flow rate from i th column
D	recycle process with direct separation sequence (without heat integration)
DB	recycle process with direct separation sequence under backward heat integration
DF	recycle process with direct separation sequence under forward heat integration
D_i	distillate flow rate from i th column
F	flow rate out of the reactor
F_{0i}	fresh feed flow rate of i th component

Fig. 16. Closed-loop responses for -8% and -11% feed composition (z_{0B}) changes with: (A) DF configuration; (B) IB configuration; and (C) direct sequence without heat integration (D).

Fig. 16. continued.

I	recycle process with indirect separation sequence
IB	recycle process with indirect separation sequence under backward heat integration
IF	recycle process with indirect separation sequence under forward heat integration
k	specific reaction rate
L_i	liquid flow rate in the column
NC	number of component
NF_i	feed tray number in column i
NT_i	total number of trays in column i
P^{sat}	vapor pressure
rr_i	reflux ratio of i th column
rxn	total reaction rate (Eq. (1))
RR_i	recycle ratio in column i
T	temperature
TAC	total annualized costs
V_i	vapor boilup in column i
V_R	reactor holdup in moles
$x_{Bk,j}$	bottom composition in k th column (mole fraction of component j)
$x_{Dk,j}$	distillate composition in k th column (mole fraction of component j)
$z_{,j}$	reactor composition (mole fraction of component j)
$z_{,oj}$	fresh feed composition (mole fraction of component j)

Greek letters

α_j	relative volatility of component j
ΔH	heat of vaporization

Subscripts

HP	high-pressure column
LP	low-pressure column

Acknowledgements

Financial support of the National Science Council of Taiwan is gratefully acknowledged and we also thank Vincent Chang for performing some simulation runs for the recycle plants. FORTRAN programs for the recycle plants are available upon request.

Appendix A.

Shortcut design, equipment sizing, and TAC calculation

1. Use twice of the minimum number of trays (Fenske equation) for column design and the Kirkbride equation for

the feed tray locations

$$N_{T,i} = 2 \frac{\log [(x_{Di,LK}/x_{Di,HK})(x_{Bi,HK}/x_{Bi,LK})]}{\log(\alpha_{LK}/\alpha_{HK})}, \quad (\text{A.1})$$

$$N_{f,i} = 1 + \frac{N_{T,i}}{1 + (x_{Fi,HK}/x_{Fi,LK})(x_{Bi,LK}/x_{Di,HK})^2 B_i/D_i)^{0.206}}. \quad (\text{A.2})$$

2. Compute reactor diameter in ft (assume an aspect ratio of 2 and an averaged molecular weight of 66.7)

$$D_R = \left(\frac{2}{\pi} \frac{V_R \text{MW}}{\rho_{\text{avg}}} \right)^{1/3}. \quad (\text{A.3})$$

3. Calculate column diameter in ft and assuming tray spacing of 2.4 ft

$$D_{C,i} = \sqrt{\frac{1}{900\pi} \left(\frac{\text{MWR}_{\text{gas}} T}{P} \right)^{1/2} V_i^{1/2}}, \quad (\text{A.4})$$

$$L_{C,i} = 2.4 N_{T,i}, \quad (\text{A.5})$$

where $R_{\text{gas}} = 1545/144$ psia ft³/lb-mol^oR, T is the averaged column temperature in ^oR, P is the column pressure in psia, V_j is the vapor flow rate in lbmol/h.

4. Use Francis weir formula to find the height over weir ($h_{ow,i}$) in ft

$$h_{ow,i} = \left(\frac{L_i \text{MW}}{9600 \rho_{\text{avg}} D_{C,i}} \right)^{2/3}. \quad (\text{A.6})$$

5. Compute liquid tray holdup ($M_{n,i}$) in lbmol assuming a weir height of 1 inch

$$M_{n,i} = \frac{(h_{ow,i} + (1/12))(\pi D_{C,i}^2/4) \rho_{\text{avg}}}{\text{MW}}. \quad (\text{A.7})$$

6. Compute liquid hydraulic time constant (β_i) in h from

$$\beta_i = \frac{\pi D_{C,i}}{57600(h_{ow,i})^{1/2}}. \quad (\text{A.8})$$

7. Compute heat transfer areas for reboiler and condenser

$$A_{R,i} = \frac{V_i \Delta H}{U_R \Delta T_R}, \quad (\text{A.9})$$

$$A_{C,i} = \frac{V_i \Delta H}{U_C \Delta T_C}. \quad (\text{A.10})$$

Assuming $U_R = 250$ Btu/(h^oF ft²), $\Delta T_R = 30^{\circ}\text{F}$, $U_C = 150$ Btu/(h^oF ft²), and $\Delta T_C = 20^{\circ}\text{F}$.

8. Use M& S index of 950 to compute capital costs and the formula taken from Douglas (1988)

$$\begin{aligned} \text{reactor cost} &= \frac{\text{M\&S}}{280} 101.9 D_R^{1.066} L_R^{0.802} \\ &\times (2.18 + (3.67 \times 1.2)), \end{aligned} \quad (\text{A.11})$$

$$\begin{aligned} \text{column cost}_i &= \frac{\text{M\&S}}{280} 101.9 D_{C,i}^{1.066} L_{C,i}^{0.802} \\ &\times (2.18 + 3.67 \times 1.2), \end{aligned} \quad (\text{A.12})$$

$$\text{tray cost}_i = \frac{\text{M\&S}}{280} 4.7 D_{C,i}^{1.55} L_{C,i} (1.0 + 0.0 + 1.7), \quad (\text{A.13})$$

$$\begin{aligned} \text{heat exchanger cost}_i &= \frac{\text{M\&S}}{280} 101.3 (A_{R,i}^{0.65} + A_{C,i}^{0.65}) \\ &\times (2.29 + (1.35 + 0.1) 3.75), \end{aligned} \quad (\text{A.14})$$

9. Compute steam (ΔH_{steam} comes from steam table) and cooling water cost (assuming $\Delta T_{\text{CW}} = 30^{\circ}\text{F}$) from

$$\text{steam cost} = \frac{\text{CS}(\Delta H \sum V_i)}{\Delta H_{\text{steam}}}, \quad (\text{A.15})$$

$$\text{cooling-water cost} = \frac{\text{CW}(\Delta H \sum V_i)}{C_{P,\text{CW}} \Delta T_{\text{CW}}}. \quad (\text{A.16})$$

Utilities cost	Price
Saturated steam	CS (per 1000 lb)
600 psig	\$4.52
250 psig	\$3.72
150 psig	\$3.4
50 psig	\$2.8
Cooling water	CW (per 1000 gal)
90° F-water	\$0.03

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