

Application of Decomposition Methodology to Solve Integrated Process Design and Controller Design Problems for Reactor-Separator-Recycle Systems

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Abstract: This paper presents the integrated process design and controller design (*IPDC*) for a reactor-separator-recycle (*RSR*) system and evaluates a decomposition methodology to solve the *IPDC* problem. Accordingly, the *IPDC* problem is solved by decomposing it into four hierarchical stages: (i) pre-analysis, (ii) design analysis, (iii) controller design analysis, and (iv) final selection and verification. The methodology makes use of thermodynamic-process insights and the reverse design approach to arrive at the final process-controller design decisions. The developed methodology is illustrated through the design of a *RSR* system involving consecutive reactions, $A \leftrightarrow B \rightarrow C$ and shown to provide effective solutions that satisfy design, control and cost criteria. The advantage of the proposed methodology is that it is systematic, makes use of thermodynamic-process knowledge and provides valuable insights to the solution of *IPDC* problems for *RSR* systems.

Keywords: decomposition; integrated process design and controller design; graphical method; reactor-separator-recycle system.

1. INTRODUCTION

The reactor-separator-recycle (*RSR*) systems which integrate the reactor with the separation unit through a recycle stream may exhibit the snowball effect where a small disturbance in the feed flow rate will cause a very large disturbance to the recycle flow rate (Luyben, 1994). In order to avoid the snowball effect, balanced control structures were proposed in which disturbance rejection effort was equally distributed by changing both reactor holdup and recycle flow rate (Wu and Yu, 1996). However, the control problems created by the snowball effect can be avoided through reactor (volume) design (Kiss et al., 2007). Consequently, instead of managing the snowball effect using some control strategy, it is possible to avoid it through an appropriate reactor design. However, there are usually trade-offs between process design and controller design when economy is taken into consideration. To address such trade-offs, the integrated process design and controller design (*IPDC*) was proposed and several methodologies have been developed (Seferlis and Georgiadis, 2004). The solution of this *IPDC* problem can be challenging in terms of problem complexity such as huge dimension of the design space which needs to be searched. Hence this approach becomes costly with respect to computational demand. Recently, we proposed a new systematic model-based *IPDC* methodology that is capable of finding the optimal solution efficiently (Hamid et al., 2010).

The methodology was shown to provide effective solutions to *IPDC* problems of a single reactor and a single separator, as well as able to identify a feasible operational window within which the snowball effect will not appear and the reaction desired product composition will be high for the *RSR* system (Hamid et al., 2010). The objective of this paper is to extend

the application of the proposed *IPDC* methodology to design a *RSR* system involving consecutive reactions $A \leftrightarrow B \rightarrow C$. The paper is structured as follows. In Section 2, the *IPDC* problem formulation and the decomposition methodology are introduced. Then the implementation of the proposed methodology for a *RSR* system is presented and discussed in Section 3, which is followed by conclusions.

2. THE *IPDC* METHODOLOGY

2.1 Problem formulation

The *IPDC* problem is typically formulated as a generic optimization problem in which a performance objective in terms of design, control and cost is optimized subject to a set of constraints: process (dynamic and steady state), constitutive (thermodynamic states) and conditional (process-control specifications)

$$\max J = \sum_{i=1}^m \sum_{j=1}^n P_{i,j} w_j \quad (1)$$

subjected to:

Process (dynamic and/or steady state) constraints

$$dx/dt = f(\mathbf{u}, \mathbf{x}, \mathbf{d}, \boldsymbol{\theta}, Y, t) \quad (2)$$

Constitutive (thermodynamic) constraints

$$0 = g_1(\mathbf{v}, \mathbf{x}) - \boldsymbol{\theta} \quad (3)$$

Conditional (process-control) constraints

$$0 = h_1(\mathbf{u}, \mathbf{x}) \quad (4)$$

$$0 \leq h_2(\mathbf{u}, \mathbf{x}, \mathbf{d}) \quad (5)$$

$$CS = \mathbf{x} + \mathbf{u}Y \quad (6)$$

In the above equations, \mathbf{x} is the set of process (controlled) variables. \mathbf{u} is the set of design (manipulated) variables. \mathbf{d} is the set of disturbance variables, $\boldsymbol{\theta}$ is the set of constitutive variables (physical properties, reaction rates), \mathbf{v} is the set of chemical system variables (molecular structure, reaction stoichiometry, etc.) and t is the independent variable (usually time). The performance function in (1) includes design, control and cost, where i indicates the category of the objective function term and j indicates a specific term of each category. w_j is the weight factor assigned to each objective term $P_{i,j}$ ($i=1,3; j=1,2$).

(2) represents a generic process model from which the steady-state model is obtained by setting $dx/dt=0$. (3) represents constitutive equations which relate the constitutive variables to the process. (4)-(5) represent sets of equality and inequality constraints (such as product purity, chemical ratio in a specific stream) that must be satisfied for feasible operation—they can be linear or non-linear. In (6), Y is the set of binary decision variables for the controller structure selection (corresponds to whether a controlled variable is paired with a particular manipulated variable or not).

Different optimization scenarios can be generated as follows:

- To achieve process design objectives, $P_{1,j}$ is maximized. $P_{1,1}$ is the performance criteria for reactor design and $P_{1,2}$ is the performance criteria for separator design.
- To achieve controller design objectives, $P_{2,1}$ is minimized by minimizing $(dx/d\mathbf{d})$ the sensitivity of controlled variables \mathbf{x} with respect to disturbances \mathbf{d} , and $P_{2,2}$ is maximized by maximizing $(d\mathbf{u}/d\mathbf{x})$ the sensitivity of the manipulated variables \mathbf{u} with respect to controlled variables \mathbf{x} for the best controller structure.
- To achieve economic objectives, $P_{3,j}$ is minimized. $P_{3,1}$ is the capital cost and $P_{3,2}$ is the operating costs.

The multi-objective function in (1) is then reformulated as

$$\max J = w_{1,j}P_{1,j} + w_{2,1}(1/P_{2,1}) + w_{2,2}P_{2,2} + w_{3,j}(1/P_{3,j}) \quad (7)$$

2.2 Decomposition-based Solution Strategy

The work flow and steps involved in the decomposition based solution strategy is shown in Fig.1 Accordingly the *IPDC* problem is decomposed into four sequential stages: (1) pre-analysis; (2) design analysis; (3) controller design analysis; and (4) final selection and verification. As shown in Fig. 1, the set of constraint equations in the *IPDC* problem is decomposed into four sub-problems which correspond to four hierarchical stages. In this way, the solution of the decomposed set of sub-problems is equivalent to that of the original problem. Detail descriptions of these four stages can be found in Hamid et al. (2010).

In the pre-analysis stage, the concepts of attainable region (*AR*) (Glasser et al., 1987) and driving force (*DF*) (Gani and Bek-Pedersen, 2000) are used to locate the optimal process-controller design solution. The design decisions are made both for the process and the controller at the maximum point of *AR* for reactors and *DF* for separators, respectively. Using

this as the starting point, all other details of the process and the controller designs are worked out using the proposed methodology (see Fig. 1). From a process design point of view, the maximum point of *AR* corresponds to the highest selectivity of the product with respect to limiting and/or selected reactant for a reactor, and the maximum point of *DF* corresponds to the lowest energy required for the separator. From a controller design point of view, at these points the controllability of the process is also best satisfied. In other words, the value of $dx/d\mathbf{d}$ is minimum and the value of $d\mathbf{u}/d\mathbf{x}$ is maximum at the corresponding maximum points at *AR* and *DF* diagrams respectively. Minimum value of $dx/d\mathbf{d}$ means the sensitivity of the controlled variables with respect to disturbance is lower. Hence, the process is more robust in maintaining its controlled variables at the optimal set points in the presence of disturbances. On the other hand, the maximum value of $d\mathbf{u}/d\mathbf{x}$ will determine the best pair of the controlled-manipulated variables (the best controller structure). Therefore, by locating the maximum point of the *AR* and *DF* as design targets, insights can be gained in terms of controllability, and the optimal solution of the process-controller design can be obtained in an integrated manner.

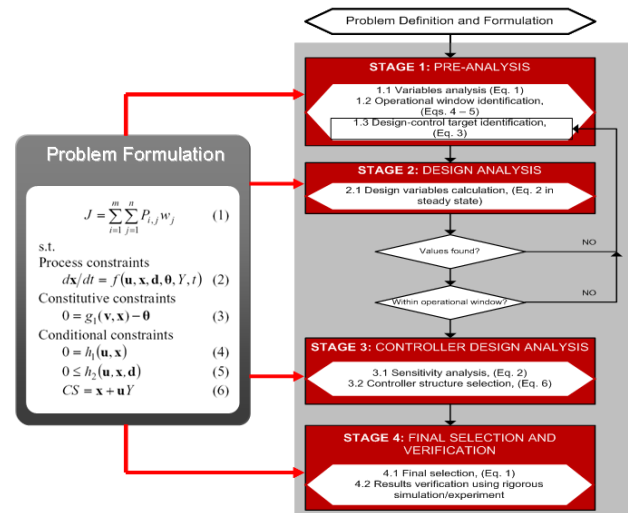


Fig. 1. Decomposition-based solution strategy for the *IPDC* problem (Hamid et al., 2010).

3. RESULTS AND DISCUSSION

This section presents the use of decomposition methodology in solving *IPDC* problem of a *RSR* system as illustrated in Fig. 2. We considered the following situation. In a continuous stirred tank reactor (*CSTR*), the product component *B* is to be produced from component *A*. Further reaction produces by-product component *C* from *B*. The reaction scheme for this system is



The value of kinetic data are assumed to be $k_1 = 306 \text{ min}^{-1}$, $k_2 = 6.6 \text{ min}^{-1}$, and $k_{-1} = 100 \text{ min}^{-1}$. We assume the effect of temperature on kinetic is negligible within the operating range. The pure component properties are tabulated in Table 1.

Table 1 Pure component properties.

Property	A	B	C
M_w (g/mol)	100.24	100.24	100.24
T_c (K)	540.2	530.37	520.5
P_c (atm)	27.042	26.98	27.37
V_c (m ³ /kmol)	0.43	0.42	0.42
T_m (K)	182.57	154.9	149.35
T_b (K)	371.58	363.20	352.34
$H_{combust}$ (kJ/kmol)	-4464730	-4459580	-4450820
Antoine equation			
A	7.10	7.20	7.08
B	1381.68	1429.67	1342.79
C	228.79	239.77	239.50

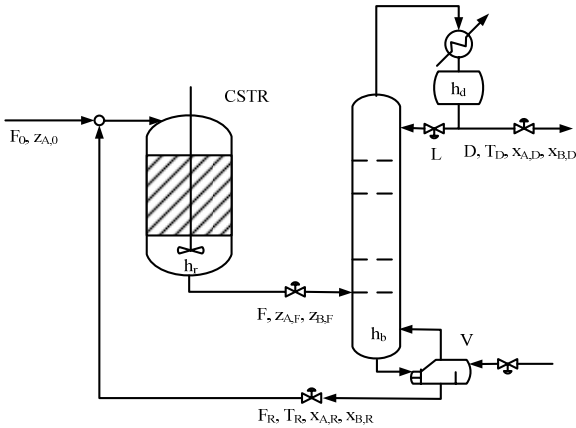


Fig. 2. RSR flowsheet with a recycle of the distillation bottom flow rate.

The feed conditions for this process are tabulated in Table 2. The objective of the reactor is to produce component B ($z_{B,F}$) as higher as possible, while the objective of the column is to keep 99% of component A in the bottom ($x_{A,R}$) (and 1% of component A in the top, $x_{A,D}$), i.e., $\mathbf{x}_I = [z_{B,F} \ x_{A,D} \ x_{A,R}]$. The reactant-rich stream F_R is recycled back to the reactor to increase the conversion. The main disturbances for reactor are the feed flow rate (F_0) and feed composition ($z_{A,0}$), i.e., $\mathbf{d}_R = [F_0 \ z_{A,0}]$, whereas the main disturbances for column are reactor effluent temperature (T), and component B ($z_{B,F}$), i.e., $\mathbf{d}_C = [T \ z_{B,F}]$. The objective here is to determine the IPDC solution in which the multi-objective function (7) is optimal—that is to produce higher and controllable product B and also to avoid the so-called snowball effect.

Table 2 Feed conditions for a RSR system.

Variables	Value	Description
F_0	60 kmol/min	Feed flow rate
$z_{A,0}$	1.0 mole fraction A	Component A composition
T	433 K	Feed temperature
P	6 atm	Feed pressure

3.1 Stage 1: Pre-analysis.

Step 1.1: Analysis of variables

The first step in stage 1 is to perform variables analysis. The important design-process variables are tabulated in Table 3. These variables are selected since they are related to the objective function (1). As shown in Fig. 2, five manipulated variables are available: reactor effluent (F), reflux flow (L), vapour boilup (V), product flow (D), and recycle flow (F_R),

hence $\mathbf{u}_0 = [F \ L \ V \ D \ F_R]$. As we need to control two liquid levels (condenser level h_d by manipulating D and column bottom level h_b by manipulating F_R) to stabilize the column (which consumes two degrees of freedom), we are left with three control degrees of freedom available for primary (composition) control, \mathbf{x}_I , which are here selected as $\mathbf{u} = [F \ L \ V]$.

Table 3 Analysis of design and process variables.

Important Design Variables
Reactor volume V_r ; Recycle F_R ; Product flow D ; Reactor effluent F ; Column stages N_S ; Column feed stage N_F ; Reflux ratio RR (Reflux L); Reboil ratio RB (Vapour boilup V); Column heat duties (Q_c and Q_r);
Important Process Variables
Reactor composition A $z_{A,F}$; Reactor composition B $z_{B,F}$; Column Bottom composition A $x_{A,R}$; Column bottom composition B $x_{B,R}$; Column bottom temperature T_R ; Column distillate composition B $x_{B,D}$; Column distillate composition A $x_{A,D}$; Column distillate temperature T_D

Step 1.2: Operational window identification

The operational window is identified based on bottom and top products purity in the column. In order to satisfy products purity, the composition of component A in the bottom should be more than 0.99 (and less than 0.01 in the top).

Step 1.3: Optimal design-control target identification

The AR diagram is generated by plotting the response of the desired product $z_{B,F}$ with respect to the response of reactant $z_{A,F}$ as shown in Fig. 3(a). Fig. 4(a) shows the plot of DF against composition for distillation design. The target for the optimal process-controller design solution is then identified at the maximum point of the AR (point A) for a reactor and the DF (point D) for distillation. Note that, in Fig. 3(a), two other points which are not at the maximum are identified as candidate alternative designs for a reactor which will be used for verification purposes (see stage 4).

Stage 2: Design Analysis.

Step 2.1: Design variables calculation.

Before calculating the value of design variables, it is important to define the feasible range of operation with respect to manipulated (design) and controlled (process) variables within which the snowball effect will not appear and desired product composition will be high. By using process model and (4), the set of conditional constraints is derived for the RSR system. Through manipulation of the mass balance equations, the set of conditional constraints are obtained in terms of dimensionless variable (Damköhler number, $Da = k_1 C_{A,F} V / F$). The dimensionless equations with respect to F_R and reactor effluent compositions ($z_{i,F}$) are obtained and solved. Results are plotted in Fig. 5.

In Fig. 5(a), it can be observed that higher value of $z_{B,F}$ can be achieved within the range of $2 < Da < 50$ (Zone II). But, when $Da < 2$ (Zone I), the F_R increases significantly indicating a possible of the snowball effect, as shown in Fig. 5(b). In order to avoid the snowball effect, the reactor should be operated at the higher value of Da (for example $Da > 2$).

However, for large values of $Da > 50$ (Zone III), there is more $z_{C,F}$ in the reactor. Therefore, for the higher $z_{B,F}$ and also to eliminate the snowball effect, the feasible operational window for Da is identified within the range of $2 < Da < 50$.

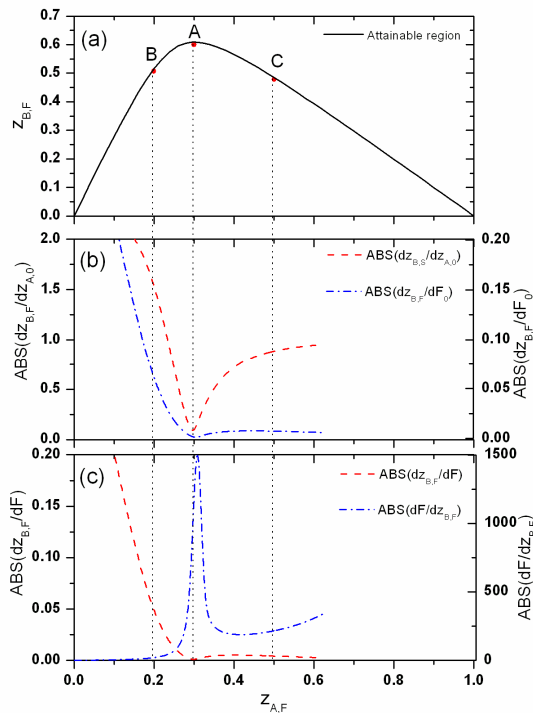


Fig. 3 (a) AR diagram for the desired product composition $z_{B,F}$ with respect to $z_{A,F}$, (b) Corresponding derivatives of $z_{B,F}$ with respect to disturbances ($z_{A,0}$ and F_0), (c) Corresponding derivatives of manipulated variable with respect to controlled variable.

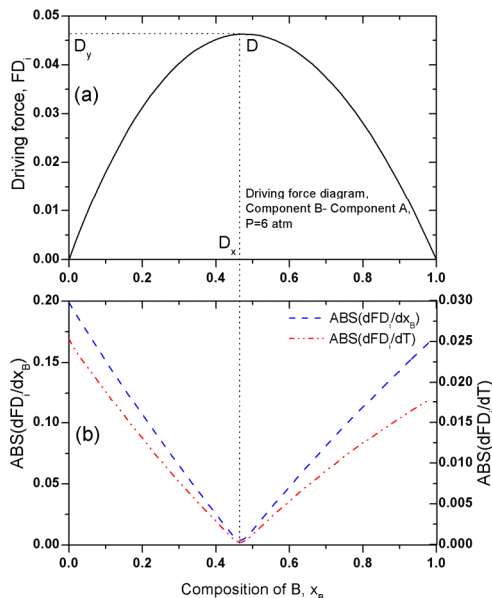


Fig. 4 (a) DF diagram for the separation of components B and A by distillation, (b) Corresponding derivatives of the DF with respect to composition and temperature.

Once the feasible range of Da has been established, process-controller design targets identified earlier at the maximum points of AR and DF, for reactor and separator designs,

respectively, are used to determine the remaining design variables and controller structure design. The results are given in Table 4 and Table 5 for reactor and distillation, respectively.

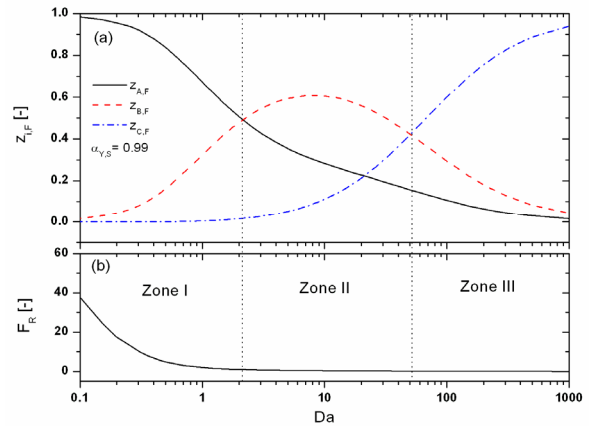


Fig. 5. Operational windows for: (a) reactor outlet composition and (b) recycle flow rate F_R as a function of Da number.

Table 4 Values of process/controlled and design/manipulated variables at different reactor designs.

Reactor design	Process/controlled		Design/manipulated			
	$z_{A,F}$	$z_{B,F}$	F (kmol/min)	F_R (kmol/min)	V (m ³)	Da
A	0.30	0.61	71.6	25.5	1.6	8.2
B	0.21	0.53	67.3	15.5	5.1	26.0
C	0.50	0.48	84.6	59.3	0.4	2.0

From Table 4, it can be seen that values of reactor volume and corresponding flow rates can be obtained for these three candidate reactor designs. In Table 5, values of distillation design variables corresponding to the maximum point of DF (point D) for three different reactor designs are obtained.

Table 5 Values of process/controlled and design/manipulated variables for distillation at point D for different reactor designs.

Reactor Design	Process/controlled					
	$x_{A,D}$	$x_{B,D}$	$x_{A,R}$	$x_{B,R}$	T_D (K)	T_R (K)
A	0.01	0.87	0.99	0.01	436.3	446.6
B	0.01	0.67	0.99	0.01	434.1	446.6
C	0.01	0.91	0.99	0.01	438.0	446.6
Reactor Design	Design/manipulated					
	N_S	N_F	L (kmol/min)	V (kmol/min)	Q_c (kJ/min) $\times 10^6$	Q_r (kJ/min) $\times 10^6$
A	65	34	730.8	337.5	-2.35	2.37
B	65	34	730.8	204.7	-2.33	2.34
C	65	34	730.8	784.3	-3.40	3.43

In Table 4, reactor design A has the highest product composition $z_{B,F}$, followed by reactor designs B and C. However, in terms of capital cost, reactor design C has the lowest cost since it has the smallest volume followed by reactor designs A and B. The distillation capital costs for three reactor designs are the same since they have the same number of stages. However, in terms of operating cost for

recycle (see Table 4) and heat duties for condenser and reboiler (see Table 5), reactor design B has the lowest cost since its recycle flow rate and heat duties are small (reactor design C has the highest operating costs while reactor design A has moderate operating costs). To find the best alternative, multi-objective function is calculated in the verification stage (see stage 4).

Stage 3: Controller Design Analysis.

Step 3.1: Sensitivity analysis.

The process sensitivity is analyzed by calculating the derivative values of the controlled variables with respect to disturbances dx/dd with a constant step size. Fig. 3(b) shows plots of derivative of $z_{B,F}$ with respect to $z_{A,0}$ and F_0 at different reactor designs. It can be seen that the derivative values are smaller for reactor design A compared to other designs (B and C). Fig. 4(b) shows plots of derivative of DF with respect to composition of B and temperature. It can be seen that derivative values are smaller at the maximum point of DF . Hence, from a control point of view, reactor design A and column design D are less sensitive to the effect of disturbances, which makes them more robust in maintaining their controlled variables against disturbances. As shown in Fig. 4(b), the value of $dz_{B,F}/dz_{A,0} = (dz_{B,F}/dh)(dh/dz_{A,0}) \approx 0$ and $dz_{B,F}/dF_0 = (dz_{B,F}/dh)(dh/dF_0) \approx 0$, thus from a control perspective, composition and level control are feasible for reactor design. For distillation design, as shown in Fig. 4(b), the value of $dFD_i/dT = dFD_i/dx_B \approx 0$, thus composition and temperature control are feasible. At the highest AR point (design A) and DF point (design D), the controller performance will be the best. At these points, any big changes to the disturbances will result in smaller changes in the controlled variables. Therefore, at these points the desired controlled variables can more easily be controlled at their optimal set points. This is verified in step 4.2.

Step 3.2: Controller structure selection.

Next the controller structure is selected by calculating the derivative value of manipulated variables with respect to controlled variables du/dx . Since there is only one manipulated variable (F) available for controlling $z_{B,F}$ and h_r for reactor design, therefore $z_{B,F}$ and h_r can be controlled by manipulating F . The value of $dF/z_{B,F}$ is calculated and plotted in Fig. 3(c). It can be seen that value of $dF/z_{B,F}$ at the maximum AR point is higher. Therefore, reactor design A requires less control action in order to maintain $z_{B,F}$ at its set point, whereas reactor designs B and C will require some additional control effort (see step 4.2). As a result, the controller structure is identified and shown in Table 6. It should be noted that, the objective of this step is not to find the optimal value of controller parameters or type of controller, but to generate the feasible controller structures.

Table 6 Proposed control structure for a RSR system.

	Reactor	Bottom	Distillate
Primary controlled variable (CV1)	$z_{B,F}$	$x_{A,R}$	$x_{A,D}$
Secondary controlled variable (CV2)	h_r	T_R	T_D
Manipulated variable (MV)	F	V	L
CV1 set point	0.61	0.99	0.01
CV2 set point	1.6m	446.6K	436.3K

Stage 4: Final Selection and Verification.

Step 4.1: Final selection: verification of design.

The multi-objective function (7) is calculated by summing up each objective function value using equal weights. This is given in Table 7. $P_{1,1s}$ corresponds to the scaled value of $z_{B,F}$. $P_{2,1s}$ and $P_{2,2s}$ are the scaled value of $dz_{B,F}/dz_{A,0}$ and $dF/dz_{B,F}$, represent process sensitivity and process gain, respectively. Whereas, $P_{3,1s}$, $P_{3,2s}$, $P_{3,3s}$ and $P_{3,4s}$ are the scaled value of reactor volume, recycle flow rate, condenser and reboiler duties, respectively, which represent capital and operating costs. It can be seen that, value of J at reactor design A is higher than other designs. Therefore, it is verified that the optimal solution for process-controller design of a RSR system which satisfies the design, control and cost criteria is given at reactor design A.

Table 7 Objective function calculation. The best candidate is highlighted in bold.

Point	$P_{1,1s}$	$P_{2,1s}$	$P_{2,2s}$	$P_{3,1s}$	$P_{3,2s}$	$P_{3,3s}$	$P_{3,4s}$	J
A	1.00	0.01	1.00	0.32	0.43	0.94	0.93	105
B	0.87	0.24	0.06	1.00	0.26	0.93	0.92	12
C	0.79	1.00	0.20	0.08	1.00	1.00	1.00	18

P_{ijs} = scaled value

Step 4.2: Closed loop dynamic simulation: verification of controller performance.

In this closed loop simulation, we use the conventional control structure (control of reactor level by manipulating F , and control of both column product compositions) to verify results obtained in the previous steps in terms of controller performance. It is assumed that the bottom and distillate compositions of the distillation are perfectly controlled, as we want to focus on the effect of the recycle to the system. Hence the reactor control structure/strategy is analyzed in detail here (see Fig. 6) to obtain controllable desired product as well as to eliminate the snowball effect. Values of tuning parameters are calculated using Ziegler-Nichols tuning method for all reactor design alternatives.

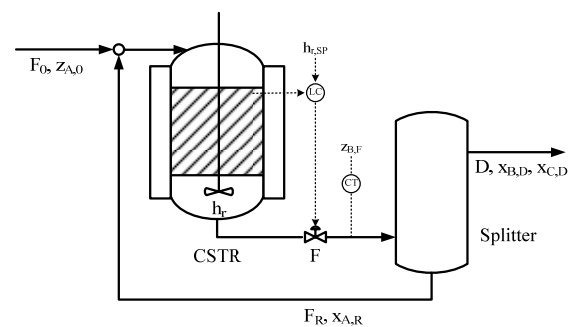


Fig. 6. Schematic diagram of reactor/distillation column plant with perfect control of both column bottom and top levels and both column product compositions.

As mentioned by Luyben (1994), the conventional control structure as shown in Fig. 6 exhibited the snowball effect. We also obtained the snowball effect when a +5% step change is applied to the F_0 (results not shown). However as proposed by Wu and Yu (1996), this snowball effect can be eliminated

by changing both reactor holdup and recycle flow rate. In the conventional control structure, it is not possible to change the recycle flow rate since it is already manipulated to control h_b . Therefore, we implemented the strategy to change the reactor holdup by allowing the reactor level controller set point to change. Fig. 7 shows the closed loop dynamic responses in $z_{B,F}$, reactor level h_r and recycle flow F_R to a +5% step increase in the F_0 .

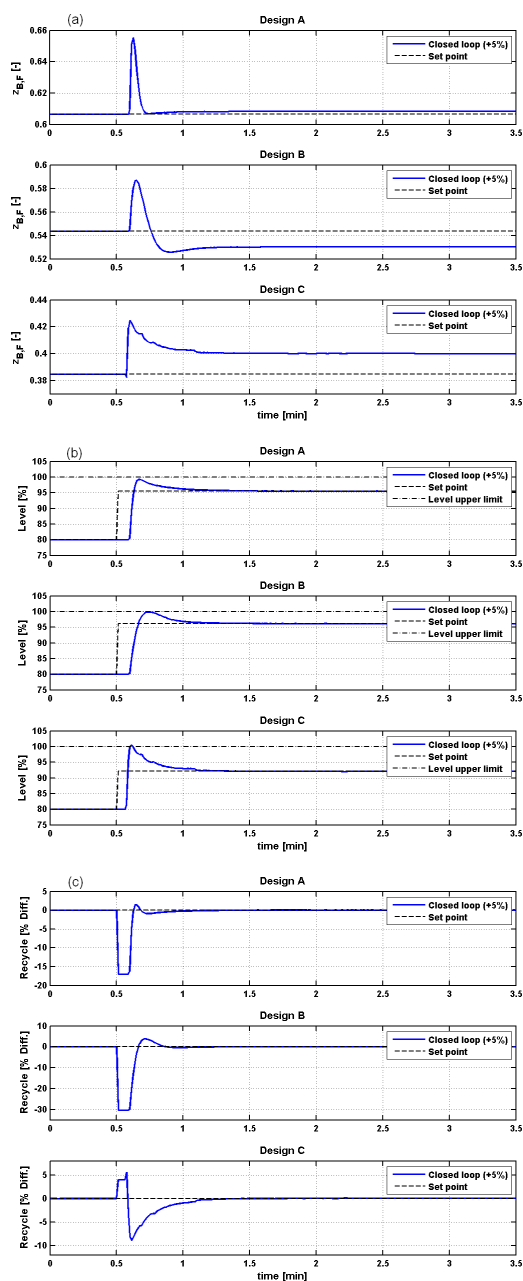


Fig. 7. Closed loop dynamic responses of (a) desired product composition $z_{B,F}$, (b) reactor level h_R , and (c) recycle flow rate F_R to a +5% step change in the F_0 for different alternative reactor designs.

One can clearly see that by allowing the reactor level set point to change at a certain value of ΔSP (Fig. 7(b)) is able to keep the recycle flow rate constant (Fig. 7(c)) for all reactor designs in the presence of disturbance. It can also be observed that the offset of the desired product composition

$z_{B,F}$ is smaller in the reactor design A (Fig. 7(a)) where other designs are showing larger offset. These results show that the $z_{B,F}$ is less sensitive to the effect of the disturbance in the reactor design A than in other designs as mentioned in the step 3 (see Fig. 3(b)) – this response was expected as indicated by the sensitivity analysis above (Fig. 3(b)). It can also be seen that less control action is required in the reactor design A to maintain $z_{B,F}$ at its set point (Fig. 7(a)). It should be noted that, the value of ΔSP becomes one of the control parameters that need to be specified optimally for the best closed loop performance. But, this is out of the scope of this work. This concludes the verification of the optimal controller design by controller configuration.

4. CONCLUSIONS

As a conclusion, the results illustrate the potential use of decomposition-based methodology in solving *IPDC* problem of *RSR* systems. It was confirmed that by applying the developed methodology, the *RSR* system with higher productivity and controllable process can be designed. The results shown that the optimal solution for the process-controller design problem which satisfies the design, control and cost criteria can be obtained at the maximum points of *AR* and *DF* for reactor and separator designs, respectively. The methodology has advantages that it is systematic, makes use of thermodynamic-process knowledge and provides valuable insights to the solution of *IPDC* problems for *RSR* systems. The methodology uses graphical methods such as *AR* and *DF* to find optimal solutions. While this may limit its applicability to high-complexity systems, there are many engineering problems (including multi-reaction, multi-component system) that can benefit from this simple method.

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