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CONTROL STRUCTURE DESIGN FOR A REACTOR/SEPARATOR PROCESS WITH TWO RECYCLES

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Abstract: A hierarchical controller is designed for a reactor/separator system which consists of a CSTR and two distillation columns with two material recycles. In designing the lower level regulatory control layer, the overall system is divided into subunits, for which regulatory control for inventories and product compositions is designed relatively independently. The higher level coordination controller is designed so that the steady state performance is near-optimal. The coordination controller manipulates some of the interconnecting flows between the subunits, namely the two recycle flows, looking at the separator loads. Control performance is demonstrated through simulations.

Keywords: plantwide control, reactor, distillation columns, hierarchical control, optimization

1. INTRODUCTION

Reactor/separator systems are one of the most common and essential parts of chemical processes; reactants are fed to a reactor unit where the reactants are partly converted to desired products and transferred to a separator unit for purification. In most cases, the unreacted reactants are recycled back to the reactor in favor of economical and environmental reasons.

Control of such recycle systems is a challenging problem, because all the units linked by recycle streams must be accounted for simultaneously. Neglecting the effect of the recycle in control system design leads to unsatisfactory performance and in some cases instabilities may appear in the closed loop response (Papadourakis *et al.*, 1987).

One way of constructing a control system for such complicated processes may be to design one large multivariable controller. Theoretically, the optimal performance is obtained with the centralized optimizing controller, but practically it has a number of disadvantages such as high cost of modeling, difficulties in controller design and tuning, maintenance and modification (Skogestad and Postlethwaite, 1996).

A popular and practical alternative is to decompose the process vertically and horizontally to form a hierarchical and decentralized control structure. Typically, a control hierarchy consists of the higher level coordination layer and the lower level regulatory layer, and time-scale separation is often possible between the tasks of these layers. The regulatory layer may be further divided horizontally into subunits to form a decentralized system, which may improve modularity. In such a control structure, the layers are interconnected through controlled variables,

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and the main issue in the control structure design problem is how the controlled variables are selected (Skogestad, 2000).

As the simplest model process of reactor/separator systems with recycle, a liquid phase continuous stirred tank reactor (CSTR) and one distillation column with one material recycle has been extensively studied in the literature (Papadourakis *et al.*, 1987; Luyben, 1994; Wu and Yu, 1996; Larsson *et al.*, 2003; Bildea and Dimian, 2003; Monroy-Loperena *et al.*, 2004). Seki et al. (Seki and Naka, 2006) applied a hierarchical control structure to this simple system. They used one of the streams interconnecting the subunits, namely the recycle flow, as the handle of the coordination controller, and realized self-optimizing control (Skogestad, 2000). At the same time, on the basis of the time-scale separation principle of the control tasks, dynamic decoupling between the subunits was achieved by limiting the bandwidth of the coordination controller.

In this paper, the same design methodology of the hierarchical controller is applied to a slightly more complex process: a reactor and two distillation columns with two recycles shown in Fig. 1.

This paper is organized as follows. In the next section, the model process is described. In Section 3, the control structure design procedure is addressed. Then, a simulation example is given for the proposed control structure. Finally, conclusions are drawn in Section 5.

2. REACTOR/SEPARATOR PROCESS WITH TWO MATERIAL RECYCLES

2.1 Process description

The model process is a ternary system, consisting of a CSTR and two distillation columns with two recycle streams, which is adapted from the process presented by Tyreus et al.(Tyreus and Luyben, 1993).

Two fresh feed streams containing pure A and B respectively are fed to the reactor, where the

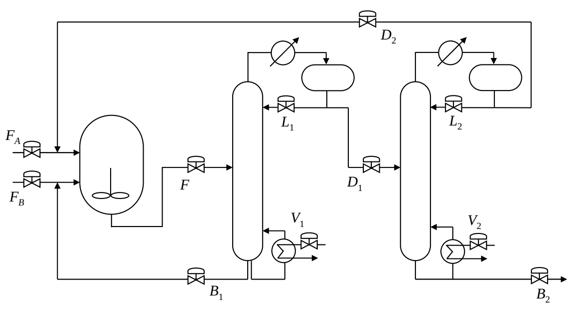

Fig. 1. Reactor/separator system with two material recycles.

Table 1. Physical properties of the hypothetical components A, B, and C

	A	B	C
Molecular weight (g/mol)	50	50	100
Density (kg/m^3)	800	800	800
Antoine constant A_j	18.93	17.43	18.12
Antoine constant B_j	-5000	-5000	-5000

Vapor pressure is calculated by the Antoine equation as $\log P_j(\text{kPa}) = A_j + B_j/T$, where T(K) is the temperature.

Table 2. Reactor data

Kinetic constant* k	0.103
Reactor holdup (m^3)	137
Fresh feed flow rate (kg/h)	2247

* Reaction rate (kmol/m^3/h) is described as $r_C = kc_Ac_B$, where c_A, c_B (kmol/m^3) are the concentrations of A and B.

Table 3. Distillation column data

	Column 1	Column 2
No. of trays	32	26
Feed stage	19	9
Feed (kg/h)	5799	5070
Vapor boilup (kmol/h)	134.7	87.6
Bottom draw (kg/h)	729	4495
Reflux (kg/h)	6951	3841
Distillate (kg/h)	5070	575
Bottom holdup (kg)	257	986
Reflux drum holdup (kg)	906	250

reaction A+B→C occurs, and the reactor effluent is sent to the distillation column trains. In the first distillation column, the heaviest component B is withdrawn from the bottom and recycled back to the reactor, while the lighter components A and C are sent from the column top to the second column. In the second column, the distillate, which is rich in the lightest component A is recycled back to the reactor, whereas the product C is withdrawn from the bottom.

The process design is based on the procedure shown by Tyreus et al. (Tyreus and Luyben, 1993) with some modifications in the distillation columns; the number of stages is calculated from Gilliland's correlation. The physical properties and basic process data are shown in Tables 1-3.

Manipulated variables are the fresh feed flows F_A and F_B, the reactor effluent F; the bottom recycle flow B_1, the vapor boilup V_1, the distillate flow D_1, the reflux flow L_1 for the first column; the bottom product flow B_2, the vapor boilup V_2, the distillate flow D_2 and the reflux flow L_2 for the second column.

Available measurements are the reactor holdup M_R; the bottom holdup $M_{B,1}$ and reflux drum holdup $M_{D,1}$ for the first column; the bottom holdup $M_{B,2}$ and reflux drum holdup $M_{D,2}$ for the second column. The composition measurements are assumed to be available at the first column top and the second column bottom, and they are denoted as $y_{i,1}$ and $x_{i,2}$, $(i = \text{A}, \text{B}, \text{C})$ respectively.

2.2 Process model

A nonlinear dynamic model is developed for control system design and simulation studies. The reactor is assumed to be well mixed and operated isothermally. For the distillation columns, the following assumptions are made: (1) constant relative volatility; (2) constant molar flows; (3) varying liquid holdup; (4) negligible vapor holdup; (5) constant pressure.

The process model, which describes the material balances, is given as ordinary differential equations in the following form:

$$\dot{x} = f(x, u), \tag{1}$$

$$y = h(x), \tag{2}$$

where $x \in \Re^{177}$ are the state variables, $u \in \Re^{11}$ are the manipulated variables and $y \in \Re^{11}$ are the measurements.

In the process model, the liquid flow rates $F_A, F_B, F, B_1, L_1, D_1, B_2, L_2$ and D_2 are given on a mass rate basis, while the vapor flow rates V_1 and V_2 are on a molar rate basis, following the convention in most applications (Jacobsen and Skogestad, 1995). In fact, use of mass based liquid flow rates results in an open loop unstable column, whose implication is discussed in some detail in the next section.

2.3 Control objective and optimal steady state operation

The control objective is a stable process operation which realizes a specified product composition and production rate with minimum energy consumption. For this purpose, the following outputs are regulated around setpoints:

$$y_R = (M_R \ M_{B,1} \ M_{D,1} \ M_{B,2} \ x_{A,2} \ x_{B,2} \ M_{D,2})^T, \tag{3}$$

where $y_R \in \Re^7$ are the subset of the measurements y.

It is assumed that the energy consumption can be approximated by the sum of the vapor boilups:

$$J = V_1 + V_2. \tag{4}$$

Then the optimal steady state operation for a specified product flow rate $\bar{B}_2$ is obtained by solving the following optimization problem:

$$\min_{x,u} J(x, u) \tag{5}$$

subject to the constraints:

$$0 = f(x, u), \tag{6}$$

$$y_R = \bar{y}_R, \tag{7}$$

$$B_2 = \bar{B}_2, \tag{8}$$

where $\bar{y}_R$ are the setpoints.

It should be noted that in the above optimization problem, the reactor holdup M_R and temperature are assumed to be constrained at their maximum. These assumptions are justified from the argument by Ward et al. (Ward *et al.*, 2004; Ward *et al.*, 2005), who showed that it is usually optimal to operate the liquid phase reactor at its maximum capacity for so-called bounded chemistries.

The optimal operation u^* is calculated for the range of $\pm 20\%$ change around the nominal production rate, which will be used for the controller design in the next section.

3. CONTROL STRUCTURE DESIGN

3.1 Basic approach

A hierarchical control structure is employed, which comprises the lower level regulatory control layer and the higher level coordination control layer. The lower level regulatory layer regulates the inventories and compositions to satisfy the constraints (7). The higher level coordination layer takes care of the remaining degree of freedom and economically optimizes process operation. In this study, self-optimizing control (Skogestad, 2000) is realized.

There are eleven manipulated variables and seven controlled variables, which implies ${}_{11}\mathrm{C}_7 = 330$ combinations for assigning the manipulated variables to the regulatory and coordination controllers. However, the number of control structure candidates can be made reasonably small, mostly on the basis of physical insight.

As the primary candidates for the coordination controller handles, the interconnecting flows between the subunits which are on the recycle paths, namely B_1 and D_2, are considered. This selection is motivated by the arguments by Ward et al. (Ward *et al.*, 2004) who advocates use of recycle streams as the operational degree of freedom. Also, by limiting the bandwidth of these manipulated variables, dynamic interactions between the subunits may be reduced (Seki and Naka, 2006).

Specification of the production rate is regarded as the task of the coordination controller, which can be conveniently done by setting either F_A or F_B on flow control. The other fresh feed flow rate cannot be put on flow control, because flow measurement inaccuracy makes it impossible to achieve perfect stoichiometric amounts of the two reactants (Tyreus and Luyben, 1993; Bildea and Dimian, 2003). Manipulation of the other fresh feed is also assigned to the coordination controller, because feed imbalance can be observed only in the plantwide context.

The basic approach in the regulatory layer design is that the whole process is divided into subunits and inventory and composition controllers are designed relatively independently for each subunit.

It should be noted that the product composition $x_{B,2}$ cannot be regulated in the second column alone; the component B is heavier than the component C, so that too much B entering the second column cannot be reduced at the bottom product flow. Regulation of $y_{B,1}$ at the top of the first column is necessary, which is regarded as the task of the regulatory controller of the first column. Then control of the product composition $x_{B,2}$ is assigned to the coordination controller, because it can be achieved only through the coordination of the two columns. Accordingly, the measurements y_R defined previously in (3) is now modified to

$$y_R = (M_R \; M_{B,1} \; M_{D,1} \; M_{B,2} \; y_{B,1} \; x_{A,2} \; M_{D,2})^T . \quad (9)$$

From these arguments, F_A, F_B, B_1, D_2 and the setpoint of the $y_{B,1}$ controller are assigned to the coordination layer, while the rest of the manipulated variables are used as the regulatory controller handles.

3.2 Regulatory control layer design

Let us begin with the second column, because this column is found to be open loop unstable and extra care should be taken for controller design. As indicated by Jacobsen et al. (Jacobsen and Skogestad, 1994), control configuration is a particularly important issue in an open loop unstable distillation column.

Typically, the bottom holdup $M_{B,2}$ is controlled by B_2, and the composition $x_{A,2}$ is controlled by V_2, while the reflux drum holdup $M_{D,2}$ is controlled either by D_2 or L_2.

In Fig.2, steady states solutions of $x_{A,2}$ and V_2 relation are compared for the cases where the top and bottom level controls are closed by (B_2, D_2) and (B_2, L_2) respectively. For the case of level control by (B_2, D_2), there exist steady state multiplicities, which implies considerable difficulties in composition control of $x_{A,2}$ by V_2. For the case of level control by (B_2, L_2), such multiplicities are eliminated. Moreover, it has been found that sufficiently tight PI level control ($M_{D,2} \leftrightarrow L_2, M_{B,2} \leftrightarrow B_2$) stabilizes the column, whereas ($M_{D,2} \leftrightarrow D_2, M_{B,2} \leftrightarrow B_2$) does not. Fortunately,

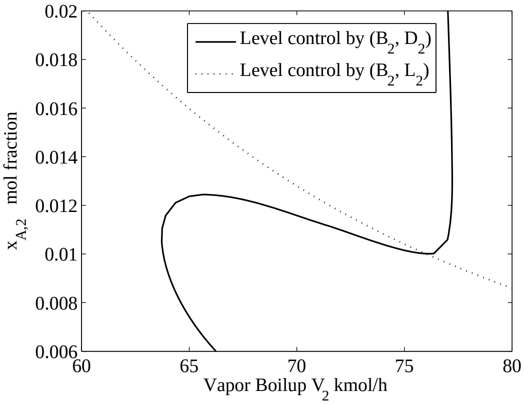

Fig. 2. Steady state relations of $x_{A,2}$ and V_2.

the reflux drum level control by L_2 does not contradict our requirement of D_2 being used by the coordination control.

For the regulatory control of the reactor, a possible control configuration is to use F to regulate the holdup M_R, because both of the recycle flows and the fresh feed flows are reserved for the coordination controller.

For the first column, a typical configuration is the bottom holdup $M_{B,1}$ controlled by V_1, since the bottom flow B_1 is used by the coordination controller. For the inventory control of the reflux drum holdup $M_{D,1}$, D_1 is the only choice, since there is a mass balance constraint: $F = D_1 + B_1$. The composition $y_{B,1}$ is controlled by the reflux L_1.

3.3 Coordination control layer design

Without coordination control, stability of the overall system is not yet guaranteed, although each isolated subunit is stabilized by the regulatory controllers. Specifically, operability is known to be very poor when the recycle flows are kept constant (Wu and Yu, 1996). In fact, the overall closed loop is found to be unstable, when controllers with integral action are used. This can be verified by the RGA analysis for the composition loops shown in Table 4, with the assumption that the level loops are closed by F, V_1, D_1, B_2 and L_2.

The coordination controller design is based on physical insight. Since the product compositions $x_{A,2}$ and $x_{B,2}$ are assumed to be regulated, the production rate may be most conveniently specified by setting one of the fresh feeds F_A or F_B on flow control. The product composition $x_{A,1}$ is

Table 4. RGA analysis for the overall process without coordination control

	Reflux L_1	Vapor Boilup V_2
$y_{B,1}$	<u>-13.2</u>	14.2
$x_{A,2}$	14.2	<u>-13.2</u>

controlled by the regulatory controller, while $x_{B,2}$ is controlled by applying cascade control from the composition measurement $x_{B,2}$ to the setpoint of the composition control for $y_{B,1}$, as shown by Tyreus et al. (Tyreus and Luyben, 1993).

The problem is how the recycle flows B_1 and D_2, and the remaining fresh feed flow should be manipulated.

Particularly, unless the distillate D_2 is appropriately manipulated under a feed increase, the second column fills up with component A, resulting in excess flow of V_2 due to the composition controller and breakthrough of A in the product stream. To prevent such a situation, the recycle D_2 should be increased and consumption of A in the reactor has to be enhanced.

Similarly, unless the bottom flow B_1 is appropriately manipulated, the first column fills up with B, resulting in excess flow of L_1. Also, any imbalance between F_A and F_B results in filling up of the component whose feed rate is larger.

The strategy is to manipulate these flows in accordance with the column loads; the recycle D_2 is manipulated according to V_2 or L_2, and the other recycle B_1 is manipulated looking at L_1 or V_1. When F_A is on flow control, F_B is manipulated according to L_1 or V_1, since excess of F_B is reflected upon too much B in the process, consequently increasing the composition controller handle L_1. Some of the candidate schemes for the coordination control configuration are shown in Table 5.

One of the simplest way to realize such coordination of the subunits would be to form ratio control between these manipulated variables. Instead of simple ratio control, the linear correlation of these variables found in the optimal operation u^* is utilized; for example, if D_2 is to be manipulated according to the column load which may be represented by V_2, the following scheme is used:

$$D_2 = aV_2 + b, \tag{10}$$

where a and b are the coefficients obtained from the linear regression for these variables in the optimal operation u^*.

Screening of the control configuration candidates To find out whether the coordination control stabilizes the overall closed loop, the same RGA analysis is applied as the one shown in Table 4. All the four candidates in Table 5 are found to be

Table 5. Candidate schemes for coordination control configuration

Scheme 1	F_A	F_B/V_2	B_1/V_1	D_2/L_2
Scheme 2	F_A	F_B/V_2	B_1/L_1	D_2/L_2
Scheme 3	F_B	F_A/L_1	B_1/V_1	D_2/L_2
Scheme 4	F_B	F_A/L_1	B_1/V_1	D_2/V_2

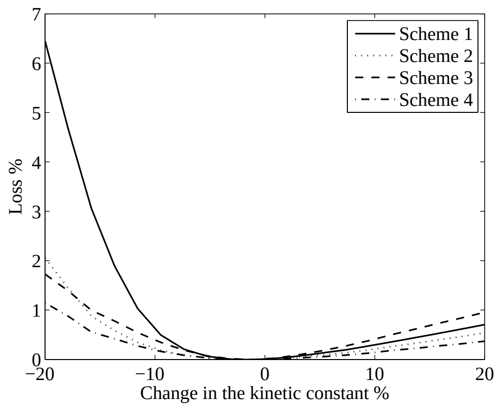

Fig. 3. Evaluation of the losses due to the kinetic constant variation.

capable of stabilizing the closed loop; the analysis result for the Scheme 1 is, for example, that the diagonal element of the RGA matrix is 0.53.

In order to discriminate the control configuration candidates, losses due to disturbances, modeling errors, and implementation errors are evaluated. For example, a model parameter is varied for $\pm 20\%$ and the energy consumption J is compared with that of the optimal operation J^*:

$$Loss\% = 100 \times (J - J^*)/J^*. \tag{11}$$

As the disturbance, a change in the production rate is considered, for which all the four candidates suffer from negligible losses. As the modeling error, a change in the kinetic constant is evaluated, and its result is shown in Fig. 3. As for the implementation errors, measurement errors in several variables are considered (Table 6). Schemes 3 and 4 are found to be comparably robust, and the Scheme 4 is employed for the following study.

Implementation of coordination control In implementing the coordination control, low pass filter is particularly useful for reducing dynamic interactions between subunits. Any disturbance occurring in one subunit can be effectively damped. The proposed control structure is shown in Fig. 4.

As indicated in Table 4, however, the closed loop becomes unstable without coordination control, which implies too slow coordination deteriorates closed loop performance. Therefore, the low pass filter time constants have to be tuned appropriately.

Table 6. Maximum losses (%) for $\pm 20\%$ implementation errors in measurements

	V_1	V_2	L_1	L_2	$x_{A,2}$	$x_{B,2}$
Scheme 1	7.3	22.9	0	11.2	3.0	6.5
Scheme 2	0	9.5	4.9	5.9	3.1	5.6
Scheme 3	3.4	0	6.1	6.2	4.3	3.8
Scheme 4	3.2	6.2	5.3	0	4.0	3.0

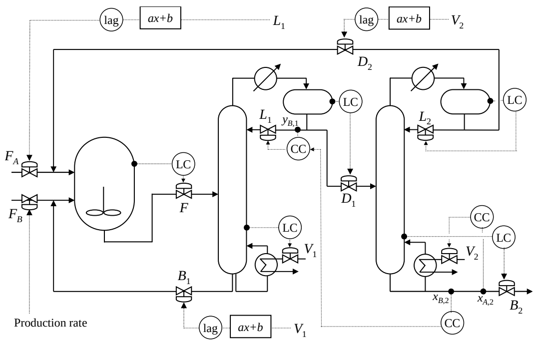

Fig. 4. Proposed control structure (Scheme 4).

4. SIMULATION

A 20% step increase in the fresh feed rate is simulated for the proposed controller. For the regulatory control layer, PI control is employed for all the loops. For the coordination control layer, the first order lag filter is applied in manipulating F_B, B_1, D_2, with filter time constant of 0.95h. For the cascade control $x_{B,2} \rightarrow y_{B,1}$, an integral control is applied with the integral time of 30min. The simulation results are shown in Fig. 5.

5. CONCLUSIONS

A hierarchical controller is designed for the reactor/separator system with two material recycles. The overall system is divided into subunits, for which the regulatory controller is designed relatively independently. The higher level coordination controller is designed in the plantwide context, which manipulates the two recycle flows to realize self-optimizing control. Feasibility of the proposed control structure has been shown through simulation.

One of the advantages of the control system design approach presented in this paper is that model identification effort may be small because detailed dynamic model is not required for control parameter calculation; PI controller tuning is all that is necessary, which can be done relatively easily.

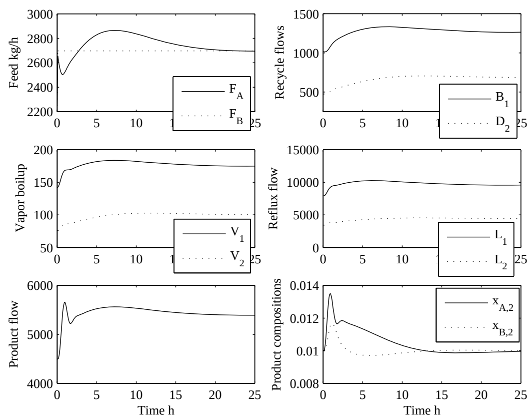

Fig. 5. Simulation results: +20% feed increase.

Constraint handling capability may be a requisite for practical applications, which may be incorporated as the task of coordination control.

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