Dynamic considerations in the synthesis of self-optimizing control structures

Journal:	*AIChE Journal*
Manuscript ID:	AIChE-07-10314.R1
Wiley - Manuscript type:	Research Article
Date Submitted by the Author:	31-Jan-2008
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Keywords:	Mathematical modeling, Optimization, Process control, Simulation, process

Dynamic considerations in the synthesis of self-optimizing control structures

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January 31, 2008

Abstract

This work builds on our prior results to develop novel control structure design principles for integrated plants featuring multiple time scale dynamics. Specifically, the concept of self-optimizing control can be used to identify the variables that must be controlled to achieve acceptable economic performance during plant operation. This approach does not, however, provide guidelines on control structure design and control loop tuning; a detailed controllability and dynamic analysis is generally needed to this end. In this work, we employ a singular perturbation-based framework, which accounts for the time scale separation present in the open loop dynamics of integrated plants, to identify the available controlled and manipulated variables in each time scale. The resulting controller design procedure thus accounts for both economic optimality and dynamic performance. The developed concepts are subsequently successfully applied on a reactor-separator process with recycle and purge.

Topical Heading: Process Systems Engineering
Keywords: Self-optimizing control, singular perturbations, dynamic analysis

Introduction

Modern chemical plant designs increasingly rely on tight integration between process units, using heat and material recycle streams, to reduce capital and operating costs. In integrated plants, economic gains come, however, at the price of an increased dynamic complexity and control challenges.

The complex dynamic behavior of integrated processes has been characterized in several works[3;4;5]. In particular, integrated processes have long been recognized to exhibit a dynamic behavior that spans multiple time scales. Many authors[6;7;8;9;10] have indirectly assumed this time scale multiplicity to propose tiered control structures, featuring at least two levels of control action: a primary layer addressing inventory and

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temperature control at the unit level and providing stability in operation, and a supervisory layer, acting over a slower time scale, that targets the control objectives at the plant level, such as product purity and production rate.

In our previous work[2], we relied on singular perturbation arguments to rigorously characterize the nonlinear dynamic behavior of integrated processes with large recycle streams and purge streams, demonstrating that it features three time scales, associated, respectively, with the evolution of the states of the individual units, with the evolution of the total material holdup of the network, and with the impurity levels in the network. We derived reduced order nonlinear models for the dynamics of the process in the three time scales, and our analysis aided in delineating a multi-tiered controller design framework, using three layers of control action to address objectives both at the unit and at the network level, using the manipulated inputs identified to be available in each time scale.

Our previous work also addressed the economic issues encountered in the operation of process networks by proposing the concept of self-optimizing control. Specifically, modern plants tend to include optimization and scheduling layers atop the supervisory control system, in order to ensure economic optimality. With this approach, however, economic performance is obtained at the price of computationally expensive real-time optimization calculations. Self-optimizing control[1] aims to alleviate this issued by identifying a set of controlled outputs which, when maintained at their setpoints, ensure that the economic losses affecting the operation of the plant in the presence of disturbances remain at an acceptable level.

The present contribution draws on our aforementioned work, utilizing the ideas in[1] to identify the controlled outputs that ensure the near-optimal operation of an integrated process that features multiple time scale dynamics. Self-optimizing control does not, however, provide information concerning the selection of the manipulated inputs to be used to control the desired outputs. In this work, rely on the analysis in[2], which accounts for the time scale separation present in the open loop dynamics of integrated plants, to identify the available controlled and manipulated variables in each time scale. The resulting controller design procedure thus accounts for both economic optimality and dynamic performance.

The paper is structured as follows: a brief description of self-optimizing control is provided in the next section, succeeded by an account of singular-perturbation based model reduction and controller design. A motivating case study is introduced, and the proposed controller synthesis approach is then presented. Finally, the newly developed framework is demonstrated via simulations.

Self-optimizing control

Self-optimizing control is defined as[1]:

Self-optimizing control is when one can achieve an acceptable loss with constant setpoint values for the controlled variables without the need to re-optimize when disturbances occur (real time optimization).

To quantify this more precisely, we define the (economic) loss L as the difference between the actual value of a given cost function and the truly optimal value, that is,

$$L(u, d) = J(u, d) - J_{opt}(d) \tag{1}$$

Truly optimal operation corresponds to $L = 0$, but in general $L > 0$. A small value of the loss function L is desired as it implies that the plant is operating close to its optimum. The central issue to self-optimizing control is not finding optimal set points, but rather finding the right variables to keep constant. The precise value of an "acceptable" loss varies from case to case, and the selection is made on the basis of engineering and economic considerations.

In[1] it is recommended that a controlled variable c suitable for constant set point control (self-optimizing control) should have the following requirements:

R1. The optimal value of c should be insensitive to disturbances, i.e., $c_{opt}(d)$ depends only weakly on d.

R2. The value of c should be **sensitive** to changes in the manipulated variable u, i.e., the gain from u to y should be large.

R3. For cases with two or more controlled variables, the selected variables in c should not be closely correlated.

R4. The variable c should be easy to measure and control.

During optimization some constraints are found to be active in which case the variables they are related to must be selected as controlled outputs, since it is optimal to keep them constant at their setpoints (active constraint control). The remaining unconstrained degrees of freedom must be fulfilled by selecting the variables (or combination thereof) which yield the smallest loss L with the active constraints implemented.

Multiple time scale dynamics of integrated process networks

In our previous work[2], we have demonstrated that the dynamic model of process networks such as that in Figure 1, featuring a reaction and a separation section that contain a recycle loop with the recycle flowrate R, and relying on a purge stream of flowrate P to eliminate any impurities present in small quantities, is captured by a stiff system of equations of the form:

$$\frac{d}{dt}\mathbf{x} = \bar{\mathbf{f}}(\mathbf{x}, \mathbf{u}^s) + \frac{1}{\varepsilon_1}\mathbf{G}^l(\mathbf{x})\mathbf{u}^l + \varepsilon_2 \mathbf{g}^P(\mathbf{x})u_p \tag{2}$$

In Equation 2, $\mathbf{x} \in \mathbb{R}^n$ is the state vector, with $\mathbf{u}^l \in \mathbb{R}^{m^l}$ being vector of scaled input variables corresponding to the flowrates of the internal streams within the recycle loop, $\mathbf{u}^s \in \mathbb{R}^{m^s}$ being the vector of scaled input variables corresponding to the flowrates of the streams outside the recycle loop (excluding the purge stream), and u_p being a scaled input variable corresponding to the flowrate of the purge stream; $\bar{\mathbf{f}}(\mathbf{x}, \mathbf{u}^s)$, $\mathbf{g}^P(\mathbf{x})$ are n-dimensional vector functions, and $\mathbf{G}^l(\mathbf{x})$ is a $n \times m^l$- dimensional matrix.

Equation 2 is developed based on the assumption that the flowrates of the recycle loop streams are are of comparable magnitude, and much higher than the network throughput, such that, at steady state, we have $\varepsilon_1 = F_{o,s}/R_s \ll 1$, and that, conversely, the flowrate of the purge stream is significantly lower than the network throughput, *i.e.*, $\varepsilon_2 = P_s/F_{o,s} \ll 1$.

Using nested singular perturbation arguments, we demonstrated that the dynamic behavior of the process network in Figure 1 features three components, that evolve over three distinct time scales. Specifically:

- a fast component, evolving in the fast time scale $\tau = t/\varepsilon_1$, described by an equation system of the form

$$\frac{d}{d\tau_1}\mathbf{x} = \mathbf{G}^l(\mathbf{x})\mathbf{u}^l \tag{3}$$

  The "stretched" time scale τ_1 is in the order of magnitude of the time constants of the individual process units with large material throughput that are part of the recycle loop, and thus the model in Equation 3 effectively captures the dynamics of thes individual process units.

- an intermediate component, evolving in the time scale t,

$$\begin{aligned} \frac{d}{dt}\mathbf{x} &= \tilde{\mathbf{f}}(\mathbf{x}, \mathbf{u}^s) + \varepsilon_2 \tilde{\mathbf{g}}^P(\mathbf{x})u_p \\ \mathbf{0} &= \tilde{\mathbf{G}}^l(\mathbf{x})\mathbf{u}^l(\mathbf{x}) \end{aligned} \tag{4}$$

  with $\mathbf{0} = \tilde{\mathbf{G}}^l(\mathbf{x})\mathbf{u}^l(\mathbf{x})$ being the linearly independent constraints that denote the quasi-steady state of the fast dynamics in the time scale t. Equation 4 is a description of the core dynamics of the process network, that is due to the presence of the recycle loop with large recycle flowrate.

- a slow component, evolving in the compressed time scale $\theta = \varepsilon_2 t$, of the general form:

$$\begin{aligned} \tfrac{d}{d\theta}\mathbf{x} &= \hat{\mathbf{g}}^P(\mathbf{x})u_p + \hat{\mathbf{B}}(\mathbf{x}) \\ \mathbf{0} &= \hat{\mathbf{G}}(\mathbf{x})\mathbf{u}^s(\mathbf{x}) \\ \mathbf{0} &= \tilde{\mathbf{G}}^l(\mathbf{x})\mathbf{u}^l(\mathbf{x}) \end{aligned} \tag{5}$$

  Note that, in Equation 5, not only the fast dynamics, but also the intermediate dynamics of the network are considered to be at a quasi-steady state. The slow component captures the dynamics associated with the presence of small amounts of feed impurity that are removed by the small purge stream.

Note that description of each of the models of the dynamics in the fast, intermediate, and slow time scales described above (respectively, Equations 3, 4, 5), features a distinct group of manipulated inputs (respectively, $\mathbf{u}^l$, $\mathbf{u}^s$ and u_p), that act upon and can be used to address control objectives in the respective time scale.

By way of consequence, process networks featuring significant material recycling, as well as a purge stream for eliminating impurities, lend themselves naturally to a hierarchical control structure, featuring three layers of control action:

- Control objectives at the unit level should be addressed in the fast time scale, using the large flowrates of the internal material streams, $\mathbf{u}^l$, as manipulated inputs.

- The control of the network wide objectives (such as product purity and production rate), should be undertaken in the intermediate time scale, using the flowrates $\mathbf{u}^s$ of the material streams outside the recycle loop as manipulated inputs

- The impurity levels in the network should be regulated using the flowrate u_p of the purge stream, over a long time horizon (slow time scale)

In the following section, we demonstrate how these results, along with the concept of self-optimizing control reviewed above, can be successfully fused in a control design procedure that accounts for both economic optimality and dynamic performance.

Case study on reactor-separator with recycle process

In this section, we present a case study that considers a reactor-separator network, interconnected via a recycle stream with a large flowrate (compared to the network throughput), and the inert impurities present in the feed are eliminated by purging. The generic process was studied in[2], and for the present paper the pressure-flow relations for the flows F, P, and R and economic data were added.

We rely on this representative example to develop and illustrate a hierarchical controller synthesis procedure, that accounts for both the time scale separation in process dynamics, and for economic criteria, in order to ensure dynamic performance and economic optimality of the closed-loop system.

Process description and modeling

The process consists of a gas-phase reactor and a condenser-separator that are part of a recycle loop (Figure 2). A low single-pass conversion requires that a large (with respect to the feed flowrate) recycle flowrate R be used in order to achieve the desired purity of the product B. The feed stream contains a small amount of an inert, volatile impurity $y_{I,o}$ which is removed via a purge stream of small flow rate P. The objective is to ensure a stable operation while controlling the purity of the product x_B.

A first-order reaction takes place in the reactor, i.e. $A \xrightarrow{k_1} B$. In the condenser-separator, the interphase mole transfer rates for the components A, B, and I are governed by rate expressions of the form $N_j = K_j\alpha(y_j - \frac{P_j^S}{P}x_j)\frac{M_L}{\rho_L}$, where $K_j\alpha$ represents the mass transfer coefficient, y_j the mole fraction in the gas phase, x_j the mole fraction in the liquid phase, P_j^S the saturation vapor pressure of the component j, P the pressure in the condenser, and ρ_L the liquid density in the separator. A compressor drives the flow from the separator (lower pressure) to the reactor. Moreover, valves with openings z_f and z_p allow the flow through F and P, respectively. Assuming isothermal operation (or, equivalently, perfect temperature control), the dynamic model of the system has the form given in Table 1.

Economic approach to the selection of controlled variables: Self-optimizing control computations

Degree of freedom analysis

The open loop system has 3 degrees of freedom at steady state, namely the position of the valve at the outlet of the reactor (z_F), the position of the purge valve (z_P), and the compressor power (W_s).

Table 2 lists the candidate controlled variables considered in this example. With 3 degrees of freedom and 18 candidate controlled outputs, there are $\binom{14}{3} = \frac{14!}{3!11!} = 364$ possible ways of selecting the control configuration, which constitutes a rather large number if we consider the dimension of the problem. Therefore, in order to avoid evaluation of each one of these possible configurations, we determine whether there are active constraints during operation.

Definition of optimal operation

The following profit is to be maximized:

$$(-J) = p_L L + p_P P - p_{F_o} F_o - p_W W_s \tag{6}$$

subject to subject to

$$\begin{aligned} P_{reactor} &\leq 2000\,kPa \\ P_{separator} &\leq 1000\,kPa \\ x_B &\geq 0.8711 \\ W_S &\leq 300\,kW \\ z_F, z_P &\in [0,1] \end{aligned} \tag{7}$$

where p_L, p_P, p_{F_o}, and p_W are the prices of the liquid product L, purge P (here assumed to be sold as fuel), feed F_o, and compressor power W_s, respectively (see also Table 3 for cost-related information).

Identification of important disturbances

We will consider the disturbances and process changes listed in Table 4 below. Specifically, we account for the possibility of variations in the feed flowrate and composition (including the possibility of having a small quantity of product present in the feed), as well as for possible changes in the product purity requirement.

Optimization

Two constraints are active at the optimum throughout the calculations (each of which corresponds to a different disturbance), namely the reactor pressure $P_{reactor}$, at its upper bound, and the product purity x_B, at its lower bound (Table 5). These consume two degrees of freedom, since it is optimal to control them at their setpoint[11], leaving 1 unconstrained degree of freedom.

Unconstrained variables: Evaluation of the loss

In order to identify the remaining controlled variable, we evaluate the steady-state economic loss incurred in the presence of disturbances, when the candidate controlled variable, in addition to the two active constraints, is perfectly controlled (i.e., it is kept constant).

Table 6 shows the results of the loss evaluation. We can see that the smallest average loss was found for the liquid mole fraction of inert in the separator (x_I). This was somehow expected since its value is essentially constant throughout the optimizations shown in Table 5. However, composition measurements have large dead times and are unreliable and we therefore disregard this candidate as the potential self-optimizing variable.

Two other candidates which show smaller average losses are the recycle flow rate R and valve opening z_F, with average losses of 0.02013 and 0.01944 \$/min, respectively. Our choice is then to select the recycle flow rate R as the unconstrained (self-optimizing) controlled variable which has an acceptable loss.

In summary, by the self-optimizing approach, the primary variables to be controlled are then $y = [P_{reactor}\ x_B\ R]$ with the manipulations $u = [z_F\ z_P\ W_S]$. In addition, secondary controlled variables may be introduced to improve the dynamic behavior of the process. With these variables, a number of control configurations can be assigned and some of them will be assessed later in this paper.

Singular perturbation approach for the selection of controlled variables

According to the hierarchical control structure design proposed by[2], based on the time scale separation of the system, the variables to be controlled and their respective manipulations are given in Table 7.

In our prior work[2], economics were not a consideration. Moreover, in the above configuration the reactor pressure is employed to control the purity of the product and is evidently required and allowed to vary, which could lead, in some cases, to the violation of the operating constraints included in the present problem formulation. A simple modification that allows the pressure constraint in the reactor to be satisfied, entails controlling x_B using the separator pressure, while maintaining the reactor pressure at its setpoint. This will be discussed later in the paper.

Control configuration for optimality and dynamic performance

The objective of this study is to explore how the configurations suggested by the two different approaches can be merged to produce an effective control structure for the system. Thus, as a starting point, we employ the following two "original" configurations: Figure 3 presents the original configuration from the singular perturbation approach[2]. Figure 4 depicts the simplest self-optimizing control configuration with control of the active constraints ($P_{reactor}$ and x_B) and self-optimizing variable R.

The configuration in Figure 3 does not account for optimality and could give rise to infeasibility with respect to operating constraints on pressure. On the other hand, the structure outlined in Figure 4 does not directly control the impurity levels in the network, and employs the flowrate of the purge streams to control the product purity, a solution which, according to our previous results, could lead to poor dynamic performance. These observations will be confirmed by the simulation results presented later in this paper.

Since one usually starts by designing the regulatory control system, the most natural starting point is the configuration in Figure 3. The first evolution of this configuration is to change the pressure control from the separator to the reactor (Figure 5). In this case, both active constraints ($P_{reactor}$ and x_B) are controlled in addition to impurity level in the reactor ($y_{I,R}$).

The final modification towards buiding a self-optimizing control structure is to change the primary controlled variable from $y_{I,R}$ to the recycle flowrate R (Figure 6). The latter evolution also ensures that the compressor power is controlled around its steady-state optimal value over a longer time scale, using the flowrate of the purge stream to this end. The final control configuration is summarized in Table 8

Results and Discussion

Simulations were carried out to assess the dynamic performance of the control configurations proposed above. The tuning parameters for the controllers in each configuration are shown in Table 9. The simulation study considered two major disturbances: a 10% drop in the feed flow rate (F_o from 100 to 90 mol/min) at $t = 10$h followed by a 5% increase in the setpoint for the product purity (x_B from 0.8711 to 0.9147) at $t = 50$ h.

The results are found in Figures 7 through 10.

Based on the simulation results presented above, notice that, in the case of the original system in Figure 3, the reactor pressure rises over the $2MPa$ bound (Figure 7) when a setpoint increase for x_B occurs. The dynamic response in terms of the product purity –a key performance indicator– is, however, very good. Moreover, the above behavior is to be expected since the original configuration was based on varying the reactor pressure to control the purity of the product.

With $P_{reactor}$ controlled with a controller with integral action (configuration of Figure 5), and manipulating the condenser pressure to control the product purity, a similar dynamic response in x_B is obtained (Figure 9). This is again to be expected, since, as explained above, the structures depicted in Figures 3 and 5 are dynamically similar. Note, however, that in this case, tracking the purity setpoint as it increases at $t = 50h$ requires a significant increase in the energy consumption of the compressor (W_S exceeds, in effect, the 300kW bound imposed in the problem formulation), intuitively leading to a less than optimal profit.

The proposed self-optimizing configuration of Figure 4, whereby the controlled variables are selected based on economics, results in a rather poor dynamic performance for the controlled variable x_B as seen in Figures 8 and 11. The explanation lies in the fact that x_B is controlled by the small flow rate P (using valve position z_P), which leads to a sluggish response. Note also that obtaining a dynamic performance in terms of x_B comparable to that of the aforementioned configurations entails using a high gain controller. Considering the data in Table 9, the gain of the purity controller in the basic self-optimizing configuration is $K_c = 100$, while the gains of the purity controllers (expressed in terms of scaled variables) in the configurations discussed above are, respectively, $K_c = 8$ and $K_c = 4$. As a consequence, in the response of Figure 8, the purge flow P is significantly increased for an extended period of time.

Finally, the configuration in Figure 6 gives feasible operation with a good transient behavior and low compressor energy consumption (Figure 10).

The developments above demonstrate that the approaches proposed in our previous work [1] and [2] are complementary in developing a control configuration at the network level, that is both economically optimal and has good dynamic performance.

The controlled outputs in the configuration illustrated in Figure 6 were selected based on economic considerations, that is, i) the active constraints in the optimization calculations, and ii) the variables that ensure a minimum loss in the presence of disturbances. The input-output pairings are based on the time scale that each controlled output evolves in, and on the manipulated inputs available in the respective time scale.

Specifically, the pressure changers (valve and compressor) that determine the large internal flowrates are used for the fast regulation of the pressure/holdup in the reactor and condenser vapor phase. Subsequently, the setpoint of the condenser vapor phase pressure controller is used to control the product purity in a slower time scale. Finally, the economic analysis recommends that the original structure be modified in the slow time scale, using the small purge flowrate to regulate the recycle flow at a set value, thereby keeping the compressor power consumption constant.

Notice that the final control structure in Table 8 is not only optimal, but also in complete agreement with the control structure design framework based on singular perturbation analysis (Table 7). Specifically, the control configurations are identical in the fast time scale. Moreover, both the reactor and the condenser pressure setpoints are manipulated inputs acting in the intermediate time scale, with the former being selected in the original configuration (Figure 3) and the latter selected in the final configuration based on optimality considerations. Last, since the flowrate of the recycle stream varies in the intermediate time scale, the purge stream must be used in the slow time scale to reset the recycle flowrate.

Note also that final control configuration proposed above is in agreement with Luyben's rule of flow-controlling one of the streams in the recycle loop [12]. However, this rule should be applied with caution [13].

Conclusion

The work presented in this paper utilized our prior results to develop novel control structure design principles for integrated plants featuring multiple time scale dynamics. Specifically, the concept of self-optimizing control was employed to identify the variables that must be controlled in order to achieve acceptable economic performance during plant operation. This approach does not, however, provide guidelines on control structure design and control loop tuning. We therefore relied on our previously introduced singular perturbation-based analysis and control framework, which accounts for the time scale separation present in the open loop dynamics of integrated plants, to identify the available controlled and manipulated variables in each time scale.

Using a prototype reactor-separator process, we successfully demonstrated the development and implementation of a controller design procedure that merges the aforementioned concepts, thereby accounting for both economic optimality and dynamic performance. Numerical simulation results indicated that the resulting controller exhibited very good transient response characteristics, while maintaining the parameters of the system within the desired economic performance envelope.

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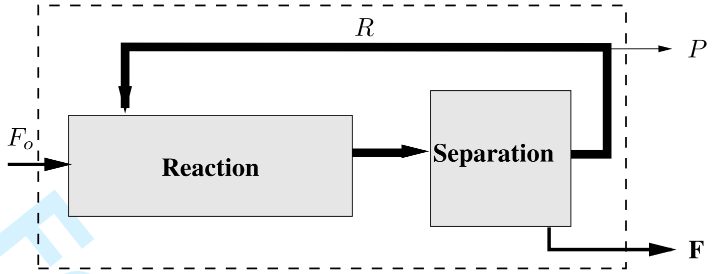

Figure 1: Generic reactor-separator process network with large recycle and purge.

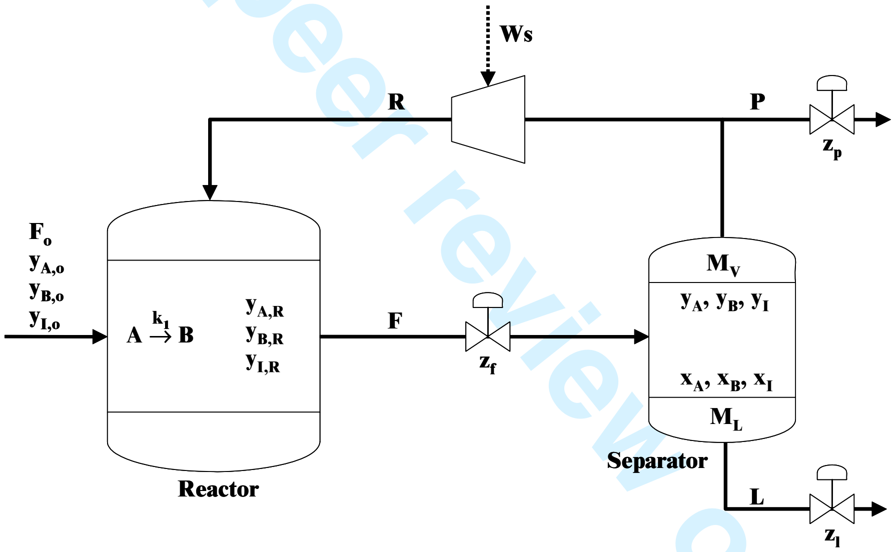

Figure 2: Reactor-separator process.

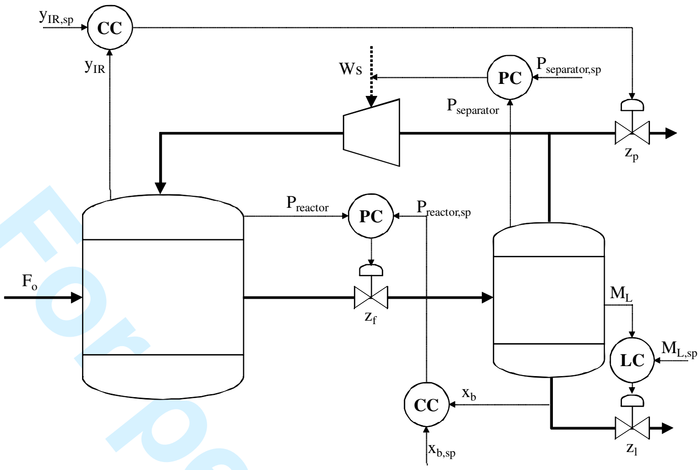

Figure 3: Original configuration based on singular perturbation with control of x_B, $P_{separator}$, and $y_{I,R}$.

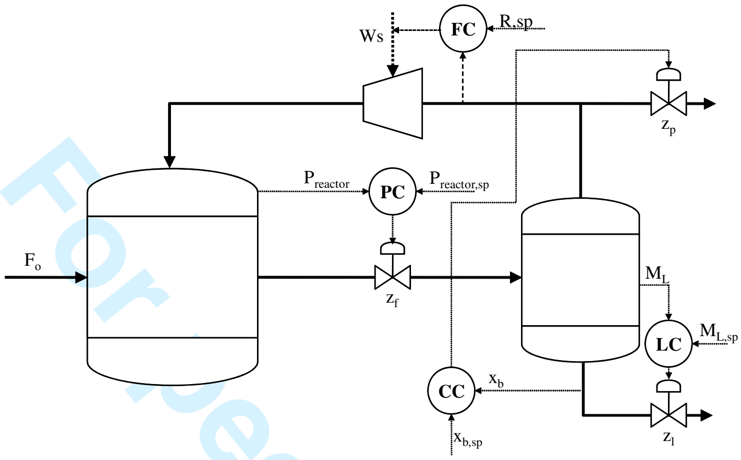

Figure 4: Simplest self-optimizing configuration with control of x_B, $P_{reactor}$, and R.

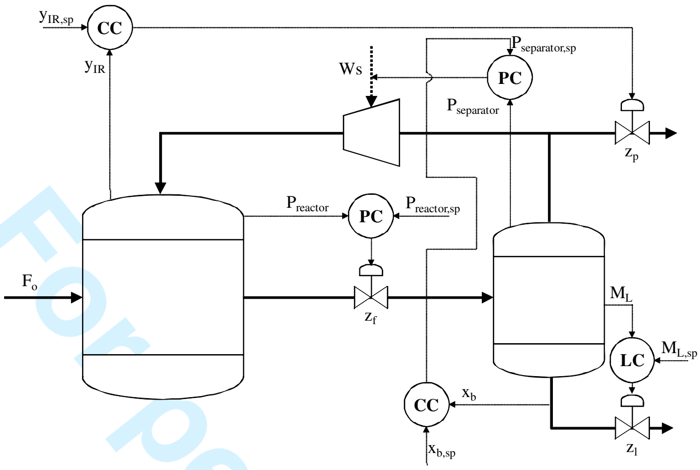

Figure 5: Modification of Figure 3: Constant pressure in the reactor instead of in the separator.

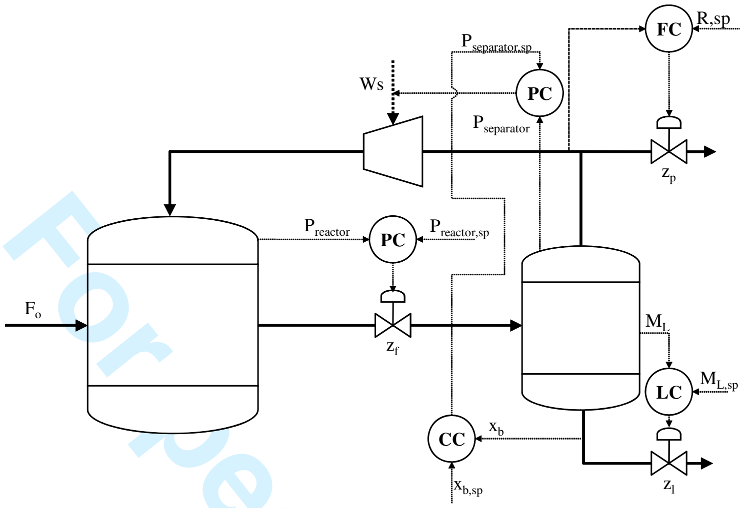

Figure 6: Final structure from modification of Figure 5: Set recycle flow rate (R) constant instead of the inert composition ($y_{I,R}$).

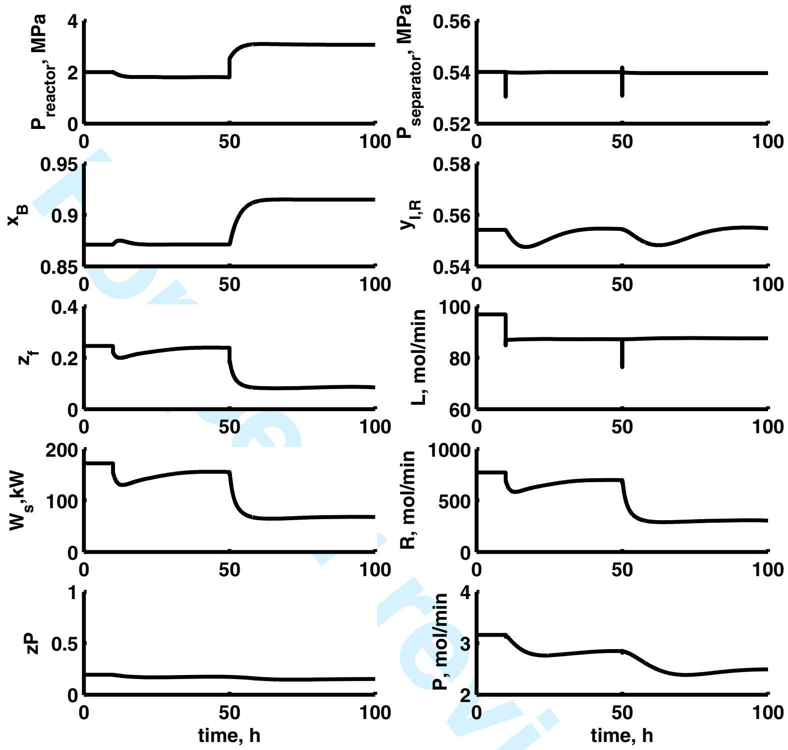

Figure 7: Closed-loop responses for configuration in Figure 3.

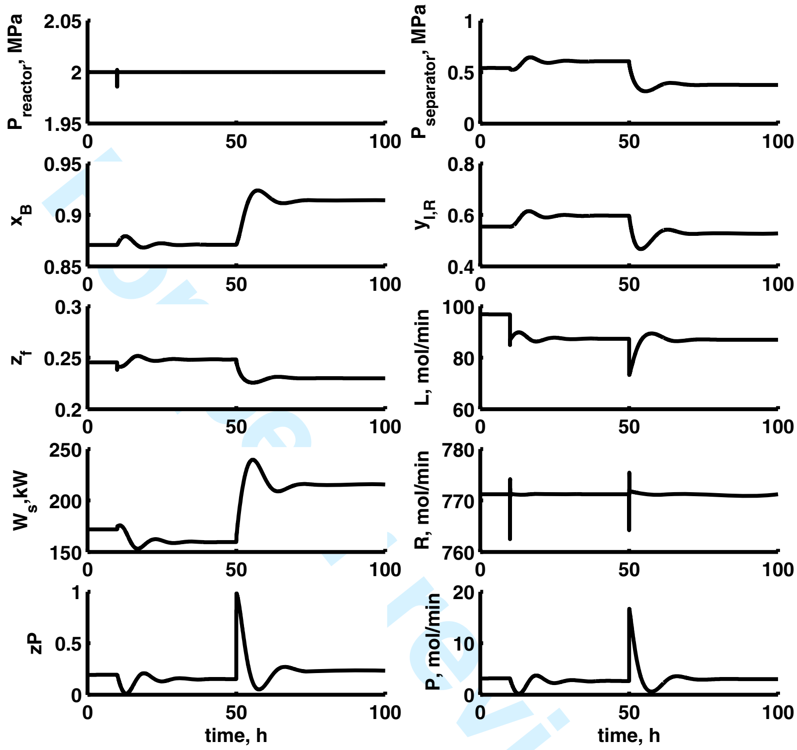

Figure 8: Closed-loop responses for configuration in Figure 4.

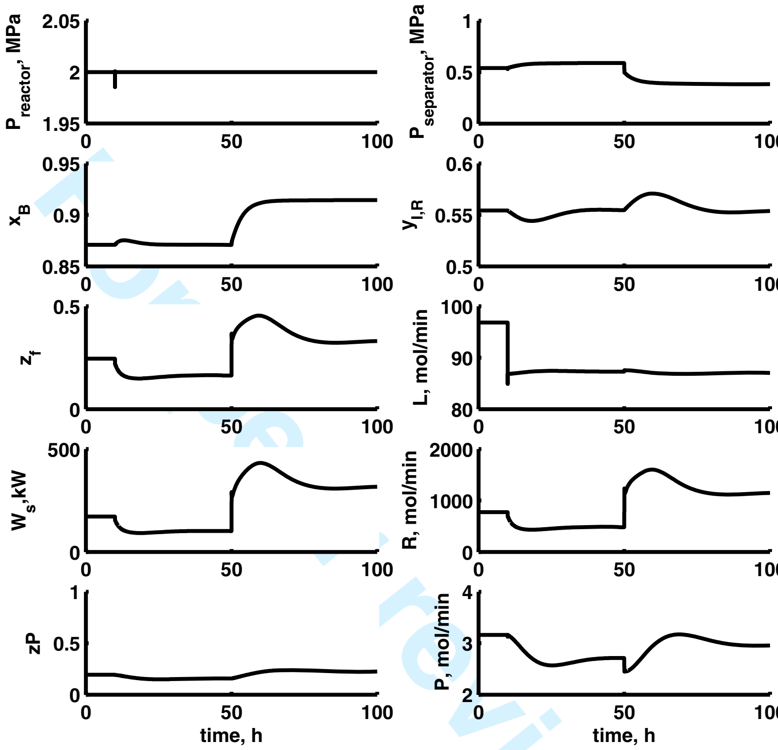

Figure 9: Closed-loop responses for configuration in Figure 5.

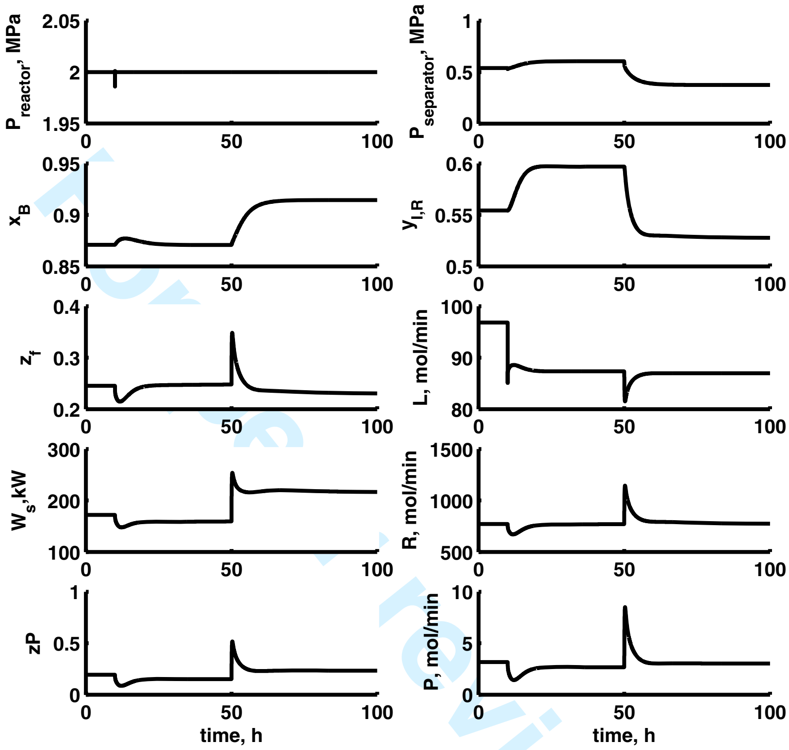

Figure 10: Closed-loop responses for configuration in Figure 6.

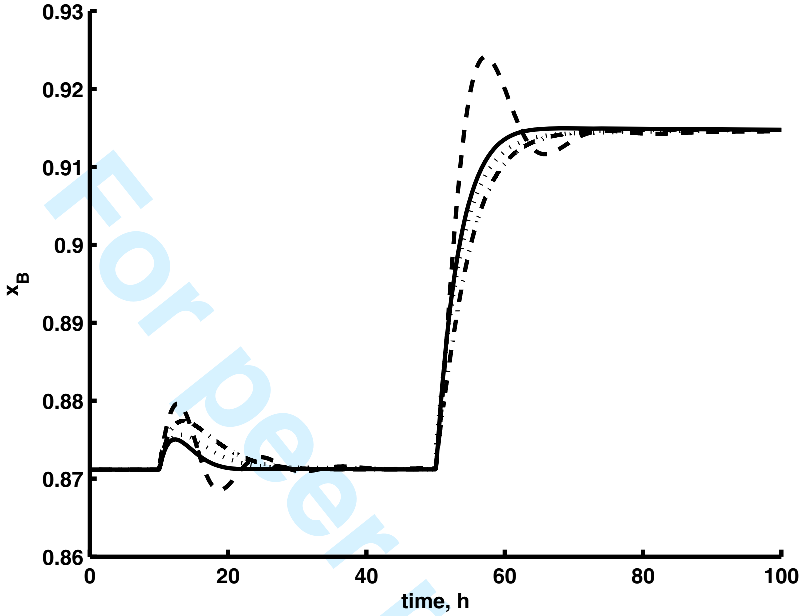

Figure 11: Closed-loop responses for the product purity x_B for the configurations in Figures 3 (solid), 4 (dash), 5 (dot) and 6 (dash-dot).

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Table 1: Dynamic model of the reactor-separator with recycle network.

Differential equations
$\frac{dM_R}{dt} = F_o + R - F$
$\frac{dy_{A,R}}{dt} = \frac{1}{M_R}[F_o(y_{A,o} - y_{A,R}) + R(y_A - y_{A,R}) - k_1 M_R y_{A,R}]$
$\frac{dy_{I,R}}{dt} = \frac{1}{M_R}[F_o(y_{I,o} - y_{I,R}) + R(y_I - y_{I,R})]$
$\frac{dM_V}{dt} = F - R - N - P$
$\frac{dy_A}{dt} = \frac{1}{M_V}[F(y_{A,R} - y_A) - N_A + y_A N]$
$\frac{dy_I}{dt} = \frac{1}{M_V}[F(y_{I,R} - y_I) - N_I + y_I N]$
$\frac{dM_L}{dt} = N - L$
$\frac{dx_A}{dt} = \frac{1}{M_L}[N_A - x_A N]$
$\frac{dx_I}{dt} = \frac{1}{M_L}[N_I - x_I N]$
Algebraic equations
$P_{reactor} = \frac{M_R R_{gas} T_{reactor}}{V_{reactor}}$
$P_{separator} = \frac{M_V R_{gas} T_{separator}}{(V_{separator} - \frac{M_L}{\rho_L})}$
$N_A = K_A \alpha \left(y_A - \frac{P_A^S}{P_{separator}} x_A \right) \frac{M_L}{\rho_L}$
$N_I = K_I \alpha \left(y_I - \frac{P_I^S}{P_{separator}} x_I \right) \frac{M_L}{\rho_L}$
$N_B = K_B \alpha \left[(1 - y_A - y_I) - \frac{P_B^S}{P_{separator}} (1 - x_A - x_I) \right] \frac{M_L}{\rho_L}$
$N = N_A + N_B + N_I$
$F = Cv_f z_f \sqrt{P_{reactor} - P_{separator}}$
$P = Cv_p z_p \sqrt{P_{separator} - P_{downstream}}$
$R = \frac{W_s}{\frac{1}{\epsilon} \frac{\gamma R_{gas} T_{separator}}{\gamma - 1} \left[\left(\frac{3 P_{reactor,max}}{P_{separator}} \right)^{\frac{\gamma - 1}{\gamma}} - 1 \right]}$

Where:
- M_R, M_V, and M_L denote the molar holdups in the reactor and separator vapor and liquid phases, respectively.
- R_{gas} is the universal gas constant.
- $\gamma = \frac{C_P}{C_V}$ is assumed constant.
- Cv_f and Cv_p are the valve constants.
- $P_{downstream}$ is the pressure downstream the system (assumed constant).
- ϵ is the compressor efficiency.
- $P_{reactor,max}$ is the maximum allowed pressure in the reactor. - The compressor and valves are modeled as first order systems, with time constants $\tau_{compressor} = 10min$ and $\tau_{valve} = 1min$.
- The flowrate L of the liquid product is assumed to be perfectly controlled.

Table 2: Selected candidate controlled variables.

Candidate	Notation
Reactor holdup (Reactor pressure)	$P_{reactor}$
Vapor mole fraction of A in the reactor	$y_{A,R}$
Vapor mole fraction of I in the reactor	$y_{I,R}$
Vapor mole fraction of A in the separator	y_A
Vapor mole fraction of I in the separator	y_I
Liquid mole fraction of A in the separator	x_A
Liquid mole fraction of I in the separator	x_I
Liquid mole fraction of B in the separator	x_B
Separator pressure	$P_{separator}$
Flow out of the reactor (Valve opening)	z_F
Liquid flow out of the separator (Valve opening)	z_L
Purge flow (Valve opening)	z_P
Recycle flow	R
Compressor power	W_S

Table 3: Prices for the components of the objective function in (6).

Price	Unit	Value
p_L	\$/mole	2.55
p_P	\$/mole	0.50
p_{F_o}	\$/mole	1.50
p_W	\$/kW	0.08

Table 4: Disturbances to the process.

		Nominal	Disturbance (Δ)
D1	Feed rate (F_o) [mole/min]	100	+20 (+20%)
D2	Feed rate (F_o) [mole/min]	100	-10 (-10%)
D3	Composition of inerts in the feed ($y_{I,o}$)	0.02	+0.004 (+20%)
D4	Product purity (x_B)	0.8711	-0.0436 (-5%)
D5	Product purity (x_B)	0.8711	+0.0436 (+5%)
D6	Composition of product B in the feed ($y_{B,o}$)	0	+0.02†

† Reduction of $y_{A,o}$ by the same amount.

Table 5: Optimization subject to the disturbances considered in Table 4.

	Unit	Nominal	D1	D2	D3	D4	D5	D6
$Profit$	\$/min	98.29	116.80	88.84	97.01	98.87	97.18	98.39
M_R	mole	6449	6449	6449	6449	6449	6449	6449
$y_{A,R}$	mole/mole	0.2625	0.3140	0.2366	0.2610	0.2496	0.2751	0.2564
$y_{I,R}$	mole/mole	0.5542	0.5023	0.5803	0.5647	0.5803	0.4970	0.5620
M_V	mole	12.36	12.01	12.32	12.32	12.31	12.30	12.32
y_A	mole/mole	0.2792	0.3323	0.2515	0.2758	0.2620	0.2934	0.2724
y_I	mole/mole	0.6234	0.5518	0.6608	0.6280	0.6730	0.5447	0.6326
M_L	mole	74150	74017	74236	74162	74406	73656	74173
x_B	mole/mole	0.8711	0.8711	0.8711	0.8711	0.8275	0.9147	0.8711
x_A	mole/mole	0.1288	0.1288	0.1288	0.1288	0.1724	0.0853	0.1288
x_I	mole/mole	0.0000557	0.0000527	0.0000555	0.0000555	0.0000554	0.0000551	0.0000554
$P_{reactor}$	Pa	2000000	2000000	2000000	2000000	2000000	2000000	2000000
$P_{separator}$	Pa	540094	453815	599573	546729	770258	340234	553578
N_A	mole/min	12.48	14.91	11.25	12.40	16.74	8.22	12.48
N_I	mole/min	0.03	0.03	0.03	0.03	0.03	0.03	0.03
N_B	mole/min	84.33	100.77	76.04	83.80	80.31	88.14	84.37
N	mole/min	96.84	115.70	87.33	96.23	97.08	96.38	96.89
F	mole/min	871.21	1289.62	716.16	954.74	704.46	1100.46	867.69
L	mole/min	96.84	115.70	87.33	96.23	97.08	96.38	96.89
P	mole/min	3.16	4.30	2.67	3.77	2.92	3.62	3.11
R	mole/min	771.21	1169.62	626.16	854.74	604.46	1000.46	767.69
z_F	-	0.25	0.36	0.20	0.27	0.21	0.30	0.24
z_P	-	0.19	0.31	0.15	0.23	0.12	0.36	0.19
W_S	kW	171.96	291.20	140.37	189.08	105.92	296.32	168.45

Table 6: Loss evaluation ($/min) for selected candidate variables based on Table 2.

Candidate	D1	D2	D3	D4	D5	D6	Avg.
$y_{A,R}$	Inf	0.36661	0.02890	0.17707	Inf	0.09963	Inf
$y_{I,R}$	Inf	0.01265	0.00456	0.00939	Inf	0.00199	Inf
y_A	Inf	0.22442	0.01111	0.12012	Inf	0.02979	Inf
y_I	Inf	0.22490	0.01116	0.37894	Inf	0.02979	Inf
x_A	0.00003	0.00000	0.01111	0.57275	Inf	0.02981	Inf
x_I	0.00003	0.00000	0.00000	0.00000	0.00009	0.00004	0.00003
$P_{separator}$	Inf	0.13732	0.01110	0.56009	Inf	0.02906	Inf
R	0.07558	0.00730	0.00263	0.00813	0.02706	0.00005	0.02013
z_F	0.07967	0.00740	0.00266	0.00512	0.02170	0.00007	0.01944
z_P	Inf	0.30234	Inf	0.54822	Inf	0.02980	Inf
W_S	0.13227	0.01391	0.00241	0.03465	0.13660	0.00006	0.05332

† Inf means infeasible operation.

Table 7: Control structure selection based on the singular perturbation analysis.

Time scale	Controlled output	Manipulation
Fast	M_R ($P_{reactor}$)	F (z_f)
Fast	M_V ($P_{separator}$)	R (z_p)
Intermediate	M_L	L
Intermediate	x_b	$M_{R,setpoint}$ ($P_{reactor,setpoint}$)
Slow	$y_{I,R}$	P

Table 8: Final control structure based on dynamic analysis and optimality.

Time scale	Controlled output	Manipulation
Fast	M_R ($P_{reactor}$)	F (z_f)
Fast	M_V ($P_{separator}$)	R (W_s)
Intermediate	M_L	L
Intermediate	x_b	$M_{V,setpoint}$ ($P_{condenser,setpoint}$)
Slow	$R(W_S)$	z_p

Table 9: Controller tuning parameters for each control configuration in Figures 3 - 6. Time constants are in minutes.

Feedback loop	Figure 3	Figure 4	Figure 5	Figure 6
$M_L \times L$	$K_c = 0.001$	$K_c = 0.001$	$K_c = 0.001$	$K_c = 0.001$
$P_{reactor} \times z_F$	$K_c = 0.001$	$K_c = 0.001$ $\tau_I = 10$	$K_c = 8$ $\tau_I = 16$	$K_c = 8$ $\tau_I = 16$
$P_{separator} \times W_S$	$K_c = 0.223$		$K_c = 0.223$	$K_c = 2.23 \cdot 10^{-3}$
$R \times z_P$				$K_c = 0.005$ $\tau_I = 1000$
$R \times W_S$		$K_c = 0.01$ $\tau_I = 2$		
$y_{I,R} \times z_P$	$K_c = 10$ $\tau_I = 500$		$K_c = 10$ $\tau_I = 410$	
$x_B \times z_P$		$K_c = 100$ $\tau_I = 1000$		
$x_B \times P_{reactor,sp}$	$K_c = 1.6 \cdot 10^7$ $\tau_I = 100$			
$x_B \times P_{separator,sp}$			$K_c = 2.16 \cdot 10^6$ $\tau_I = 100$	$K_c = 2.16 \cdot 10^6$ $\tau_I = 100$

Time scale separation and the link between open-loop and closed-loop dynamics

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Abstract

This paper aims at combining two different approaches [(Skogestad, 2000) and (Baldea and Daoutidis, 2006)] into a method for control structure design for plants with large recycle. The self-optimizing approach (Skogestad, 2000) identifies the variables that must be controlled to achieve acceptable economic operation of the plant, but it gives no information on how fast these variables need to be controlled and how to design the control system. A detailed controllability and dynamic analysis is generally needed for this. One promising alternative is the singular perturbation framework proposed in Baldea and Daoutidis (2006) where one identifies potential controlled and manipulated variables on different time scales. The combined approaches has successfully been applied to a reactor-separator process with recycle and purge.

Key words: Singular perturbation, self-optimizing control, regulatory control, selection of controlled variable.

1 Introduction

Time scale separation is an inherent property of many integrated process units and networks. The time scale multiplicity of the open loop dynamics (e.g., Baldea and Daoutidis (2006)) may warrant the use of multi-tiered control structures, and as

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Preprint submitted to Elsevier *19 October 2006*

such, a hierarchical decomposition based on time scales. A hierarchical decomposition of the control system arises from the generally separable layers of: (1) Optimal operation at a slower time scale ("supervisory control") and (2) Stabilization and disturbance rejection at a fast time scale ("regulatory control"). Within such a hierarchical framework:

a. The upper (slow) layer controls variables (CV's) that are more important from an overall (long time scale) point of view and are related to the operation of the entire plant. Also, it has been shown that the degrees of freedom (MV's) available in the slow layer include, along with physical plant inputs, the setpoints (reference values, commands) for the lower layer, which leads naturally to cascaded control configurations.
b. The lower (fast) variables implements the setpoints given by the upper layer, using as degrees of freedom (MV's) the physical plant inputs (or the setpoints of an even faster layer below).
c. With a "reasonable" time scale separation, typically a factor of five or more in closed-loop response time, the stability (and performance) of the fast layer is not influenced by the slower upper layer (because it is well inside the bandwidth of the system).
d. The stability (and performance) of the slow layer depends on a suitable control system being implemented in the fast layer, but otherwise, assuming a "reasonable" time scale separation, it should not depend much on the specific controller settings used in the lower layer.
e. The lower layer should take care of fast (high-frequency) disturbances and keep the system reasonable close to its optimum in the fast time scale (between each setpoint update from the layer above).

The present work aims to elucidate the open-loop and closed-loop dynamic behavior of integrated plants and processes, with particular focus on reactor-separator networks, by employing the approaches of singular perturbation analysis and self-optimizing control. It has been found that the open-loop strategy by singular perturbation analysis in general imposes a time scale separation in the "regulatory" control layer as defined above.

2 Self-optimizing control

Self-optimizing control is defined as:

Self-optimizing control is when one can achieve an acceptable loss with constant setpoint values for the controlled variables without the need to re-optimize when disturbances occur (real time optimization).

To quantify this more precisely, we define the (economic) loss L as the difference between the actual value of a given cost function and the truly optimal value, that is to say,

$$L(u,d) = J(u,d) - J_{opt}(d) \quad (1)$$

Truly optimal operation corresponds to $L = 0$, but in general $L > 0$. A small value of the loss function L is desired as it implies that the plant is operating close to its optimum. The main issue here is not to find optimal set points, but rather to find the right variables to keep constant. The precise value of an "acceptable" loss must be selected on the basis of engineering and economic considerations.

In Skogestad (2000) it is recommended that a controlled variable c suitable for constant set point control (self-optimizing control) should have the following requirements:

R1. The optimal value of c should be insensitive to disturbances, i.e., $c_{opt}(d)$ depends only weakly on d.
R2. The value of c should be **sensitive** to changes in the manipulated variable u, i.e., the gain from u to y should be large.
R3. For cases with two or more controlled variables, the selected variables in c should not be closely correlated.
R4. The variable c should be easy to measure and control.

During optimization some constraints are found to be active in which case the variables they are related to must be selected as controlled outputs, since it is optimal to keep them constant at their setpoints (active constraint control). The remaining unconstrained degrees of freedom must be fulfilled by selecting the variables (or combination thereof) which yield the smallest loss L with the active constraints implemented.

3 Time scale separation by singular perturbation analysis

In Baldea and Daoutidis (2006) and Kumar and Daoutidis (2002) it has shown that the presence of material streams of vastly different magnitudes (such as purge streams or large recycle streams) leads to a time scale separation in the dynamics of integrated process networks, featuring a fast time scale, which is in the order of magnitude of the time constants of the individual process units, and one or several slow time scales, capturing the evolution of the network. Using singular perturbation arguments, it is proposed a method for the derivation of non-linear, non-stiff, reduced order models of the dynamics in each time scale. This analysis also yields a rational classification of the available flow rates into groups of manipulated inputs that act upon and can be used to control the dynamics in each time scale. Specifically, the large flow rates should be used for distributed control at the unit level, in the fast time scale, while the small flow rates are to be used for addressing control objectives at the network level in the slower time scales.

In this approach it is assumed that a non-linear model of the process (usually comprising a reaction and separation section linked by a large recycle stream) is available. The principle of this method consists in rearranging and further decomposing the model according to its characteristic time scale separation found by considering the different orders of magnitude of its variables (flows). For a reactor-separator network with a large recycle flow compared with its throughput and small purge of inert components, three different time scales can be identified. In addition, during the rearrangement step two sort of inputs can be classified: those corresponding to "large" flow rates (u^l) and those corresponding to "small" flow rates (u^s).

The decomposition of the rearranged system is carried out based on the singular perturbation analysis. This step consists of finding the three equations which describe the system within the fast, intermediate, and slow time scales as well as revealing in a natural way which manipulated variables are to be used in each time scale: u^l is to manipulate the variables in the fast time scale, u^s is used to manipulate the variables in the intermediate time scale, and u_p (the purge flow rate) manipulates the small amount of feed impurity.

Thus, control objectives in each of the time scales can be addressed by using the manipulated inputs that are available and act upon the dynamics in the respective time scale, starting from the fastest. Specifically:

a. Large flow rates are available for addressing regulatory control objectives at the unit level, such as liquid level/holdup control, as well as for the rejection of fast disturbances. Similar control objectives for the units outside the recycle loop are to be addressed using the small flow rates u^s, as the large flow rates do not influence the evolution of these units. Typically, the above control objectives objectives are fulfilled using simple linear controllers, possibly with integral action, depending on the stringency of the control objectives.

b. The small flow rates u^s appear as the manipulated inputs available for controlling the "overall" network dynamics in the intermediate time scale. Control objectives at network level include the product purity, the stabilization of the total material holdup and setting the production rate. Very often, the number of available manipulated inputs u^s is exceeded by the number of network level control objectives. In this case, it is possible to use the setpoints y^l_{sp} of the controllers in the fast time scale as manipulated inputs in the intermediate time scale, which leads to cascaded control configurations. Such configurations are beneficial from the point of view of achieving a tighter coordination between the distributed and supervisory control levels.

c. The concentration of the impurities in the network evolves over a very slow time scale. Moreover, the presence of impurities in the feed stream, corroborated with the use of large recycle flow rates, can lead to the accumulation of the impurities in the recycle loop, with detrimental effects on the operation of the network and on the process economics. Therefore, the control of the impurity levels in the network is a key operational objective and it should be addressed in the slow time scale, using the flow rate of the purge stream u_p, as a manipulated input.

4 Case study on reactor-separator with recycle process

In this section, a case study on reactor-separator network is considered where the objective is to hierarchically decide on a control structure which inherits the time scale separation of the system in terms of its closed-loop characteristics. This process was studied in Kumar and Daoutidis (2002), but for the present paper the expressions for the flows F, L, P, and R and economic data were added.

4.1 The process

The process consists of a gas-phase reactor and a condenser-separator that are part of a recycle loop (see Figure 1). It is assumed that the recycle flow rate R is much larger than the feed flow rate F_o and that the feed stream contains a small amount of an inert, volatile impurity $y_{I,o}$ which is removed via a purge stream of small flow rate P. The objective is to ensure a stable operation while controlling the purity of the product x_B.

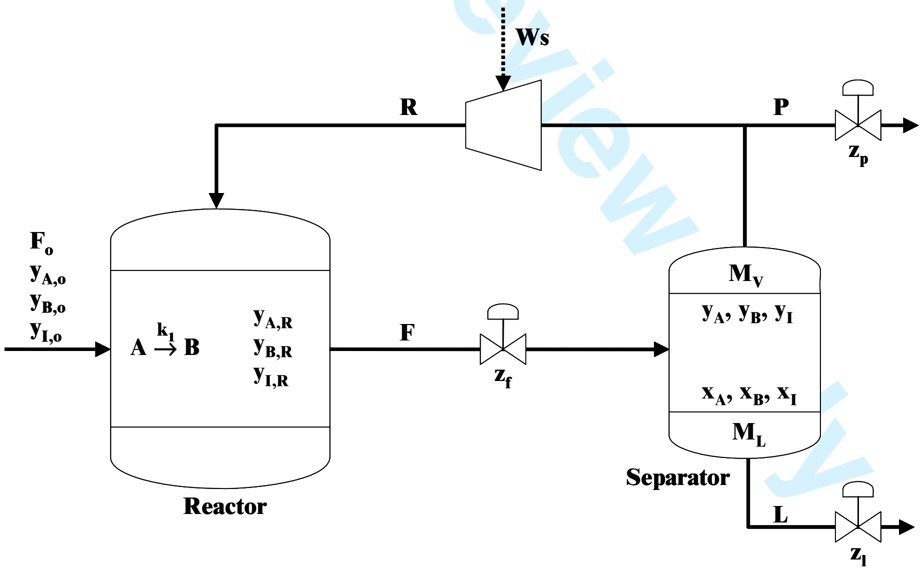

Fig. 1. Reactor-separator process.

A first-order reaction takes place in the reactor, i.e. $A \xrightarrow{k_1} B$. In the condenser-separator, the interphase mole transfer rates for the components A, B, and I are governed by rate expressions of the form $N_j = K_j\alpha(y_j - \frac{P_j^S}{P}x_j)\frac{M_L}{\rho_L}$, where $K_j\alpha$

represents the mass transfer coefficient, y_j the mole fraction in the gas phase, x_j the mole fraction in the liquid phase, P_j^S the saturation vapor pressure of the component j, P the pressure in the condenser, and ρ_L the liquid density in the separator. A compressor drives the flow from the separator (lower pressure) to the reactor. Moreover, valves with openings z_f, z_l, and z_p allow the flow through F, L, and P, respectively. Assuming isothermal operation (meaning that the reactor and separator temperatures are perfectly controlled), the dynamic model of the system has the form given in Table 1.

4.2 *Economic approach to the selection of controlled variables: Self-optimizing control computations*

4.2.1 *Degree of freedom analysis*

The open loop system has 3 degrees of freedom at steady state, namely the valve at the outlet of the reactor (z_F), the purge valve (z_P), and the compressor power (W_s). The valve at the separator outlet (z_L) has no steady state effect and is used solely to stabilize the process.

Table 2 lists the candidate controlled variables considered in this example. With 3 degrees of freedom and 18 candidate there are $\binom{18}{3} = \frac{18!}{3!15!} = 816$ possible ways of selecting the control configuration. We then determine whether there are active constraints during operation.

4.2.2 *Definition of optimal operation*

The following profit is to be maximized:

$$(-J) = (p_L - p_P)L - p_W W_s \tag{2}$$

subject to

$$\begin{aligned} P_{reactor} &\leq 2MPa \\ x_B &\geq 0.8711 \\ W_S &\leq 20kW \\ z_F, z_P &\in [0, 1] \end{aligned}$$

where p_L, p_P, and p_W are the prices of the liquid product, purge (here assumed to be sold as fuel), and compressor power, respectively.

Table 1
Dynamic model of the reactor-separator with recycle network.

Differential equations

$$\frac{dM_R}{dt} = F_o + R - F$$

$$\frac{dy_{A,R}}{dt} = \frac{1}{M_R}[F_o(y_{A,o} - y_{A,R}) + R(y_A - y_{A,R}) - k_1 M_R y_{A,R}]$$

$$\frac{dy_{I,R}}{dt} = \frac{1}{M_R}[F_o(y_{I,o} - y_{I,R}) + R(y_I - y_{I,R})]$$

$$\frac{dM_V}{dt} = F - R - N - P$$

$$\frac{dy_A}{dt} = \frac{1}{M_V}[F(y_{A,R} - y_A) - N_A + y_A N]$$

$$\frac{dy_I}{dt} = \frac{1}{M_V}[F(y_{I,R} - y_I) - N_I + y_I N]$$

$$\frac{dM_L}{dt} = N - L$$

$$\frac{dx_A}{dt} = \frac{1}{M_L}[N_A - x_A N]$$

$$\frac{dx_I}{dt} = \frac{1}{M_L}[N_I - x_I N]$$

Algebraic equations

$$P_{reactor} = \frac{M_R R_{gas} T_{reactor}}{V_{reactor}}$$

$$P_{separator} = \frac{M_V R_{gas} T_{separator}}{(V_{separator} - \frac{M_L}{\rho_L})}$$

$$N_A = K_A \alpha \left(y_A - \frac{P_A^S}{P_{separator}} x_A\right) \frac{M_L}{\rho_L}$$

$$N_I = K_I \alpha \left(y_I - \frac{P_I^S}{P_{separator}} x_I\right) \frac{M_L}{\rho_L}$$

$$N_B = K_B \alpha \left[(1 - y_A - y_I) - \frac{P_B^S}{P_{separator}}(1 - x_A - x_I)\right] \frac{M_L}{\rho_L}$$

$$N = N_A + N_B + N_I$$

$$F = Cv_f z_f \sqrt{P_{reactor} - P_{separator}}$$

$$L = Cv_l z_l \sqrt{P_{separator} - P_{downstream}}$$

$$P = Cv_p z_p \sqrt{P_{separator} - P_{downstream}}$$

$$R = \frac{W_s}{\frac{1}{\epsilon}\frac{\gamma R_{gas} T_{separator}}{\gamma - 1}\left[\left(\frac{3P_{reactor,max}}{P_{separator}}\right)^{\frac{\gamma-1}{\gamma}} - 1\right]}$$

Where:

- M_R, M_V, and M_L denote the molar holdups in the reactor and separator vapor and liquid phases, respectively.

- R_{gas} is the universal gas constant.

- $\gamma = \frac{C_P}{C_V}$ is assumed constant.

- Cv_f, Cv_l, and Cv_p are the valve constants.

- $P_{downstream}$ is the pressure downstream the system (assumed constant).

- ϵ is the compressor efficiency.

- $P_{reactor,max}$ is the maximum allowed pressure in the reactor.

Table 2
Selected candidate controlled variables.

Y1	Reactor holdup	M_R
Y2	Vapor mole fraction of A in the reactor	$y_{A,R}$
Y3	Vapor mole fraction of I in the reactor	$y_{I,R}$
Y4	Vapor mole fraction of A in the separator	y_A
Y5	Vapor mole fraction of I in the separator	y_I
Y6	Liquid mole fraction of A in the separator	x_A
Y7	Liquid mole fraction of B in the separator	x_B
Y8	Liquid mole fraction of I in the separator	x_I
Y9	Reactor pressure	$P_{reactor}$
Y10	Separator pressure	$P_{separator}$
Y11	Flow out of the reactor	F
Y12	Liquid flow out of the separator	L
Y13	Purge flow	P
Y14	Recycle flow	R
Y15	Valve opening	z_F
Y16	Valve opening	z_L
Y17	Valve opening	z_P
Y18	Compressor power	W_S

4.2.3 Identification of important disturbances

We will consider the disturbances listed in Table 3 below.

4.2.4 Optimization

Two constraints are active at the optimal through the optimizations (each of which corresponding to a different disturbance), namely the reactor pressure $P_{reactor}$ at its upper bound and the product purity x_b at its lower bound. These consume 2 degree of freedom since it is optimal to control them at their setpoint (Maarleveld and Rijnsdorp, 1970) leaving 1 unconstrained degree of freedom.

4.2.5 Unconstrained variables: Evaluation of the loss

To find the remaining controlled variable, it is evaluated the loss imposed by keeping selected variables constant when there are disturbances.

Table 3
Disturbances to the process operation.

No.	Disturbance
D1	20% increase in F_0
D2	10% reduction in F_0
D3	20% increase in $y_{I,o}$
D4	$y_{B,o} = 0.02$ with $y_{A,o} = 0.96$
D5	5% reduction in $K_{reaction}$
D6	10% reduction in $T_{reaction}$
D7	5% reduction in x_B
D8	5% increase in x_B

The candidate set is given in Table 2 with the exception of $P_{reactor}$ and x_B. Table 4 shows the results of the loss evaluation. We see that the smallest losses were found for the compressor power W_s which is then selected as the unconstrained controlled variable.

In summary, by the self-optimizing approach, the primary variables to be controlled are then $y = [P_{reactor}\ x_B\ W_S]$ with the manipulations $u = [z_F\ z_P\ W_S]$. In addition, secondary controlled variables may be introduced to improve the dynamic behavior of the process. With these variables, a number of control configurations can be assigned and some of them will be assessed later in this paper.

4.3 Singular perturbation approach for the selection of controlled variables

According to the hierarchical control structure design proposed by Baldea and Daoutidis (2006) based on the time scale separation of the system, the variables to be controlled and their respective manipulations are given in Table 5. It is important to note that no constraints are imposed in the variables in contrast with the self-optimizing control approach.

Previously in Baldea and Daoutidis (2006) economics were not considered and the structure they found leads to infeasible operation since the constraint in the reactor pressure $P_{reactor}$ (or M_R) and compressor power (W_S) can be exceeded in some cases. A simple modification would be to control x_B using the separator pressure and keeping the reactor pressure at its setpoint. This will be discussed later in this paper.

Table 4
Loss evaluation for the selected candidates in Table 2.

Candidate	D1	D2	D3	D4	D5	D6	D7	D8	Avg.
M_R	0.000	0.009	0.010	0.000	0.000	Inf$^{(*)}$	Inf	0.000	Inf
$y_{A,R}$	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf
$y_{I,R}$	Inf	2.801	2.069	5.993	0.125	6.757	Inf	Inf	Inf
y_A	Inf	Inf	11.154	Inf	Inf	68.494	Inf	34.500	Inf
y_I	Inf	5.047	11.517	61.738	Inf	68.516	Inf	Inf	Inf
x_A	Inf	0.369	0.422	3.598	Inf	1.461	Inf	Inf	Inf
x_I	Inf	0.369	0.421	3.598	Inf	1.461	Inf	1.599	Inf
$P_{separator}$	574.629	5.039	11.505	Inf	Inf	Inf	Inf	Inf	Inf
F	6.653	1.963	0.497	0.268	1.340	0.010	4.061	0.946	1.967
L	Inf	Inf	Inf	Inf	Inf	69.366	Inf	Inf	Inf
P	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf
R	6.325	1.963	0.474	0.212	1.340	0.010	4.061	1.087	1.934
z_F	5.951	2.122	0.541	0.151	1.135	0.048	0.851	0.314	1.389
z_L	Inf	Inf	Inf	Inf	Inf	69.263	Inf	Inf	Inf
z_P	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf
W_S	2.877	1.887	0.367	0.780	1.074	0.110	1.635	0.855	1.198

$^{(*)}$ Inf means infeasible operation.

Table 5
Control structure selection based on the singular perturbation analysis.

Time scale	Controlled output	Manipulation
Fast	M_R ($P_{reactor}$)	F (z_f)
Fast	M_V ($P_{separator}$)	R (z_p)
Intermediate	M_L	L (z_l)
Intermediate	x_b	$M_{R,setpoint}$ ($P_{reactor,setpoint}$)
Slow	$y_{I,R}$	P

4.4 *Control configuration arrangements*

The objective of this study is to explore how the configurations suggested by the two different approaches can be merged to produce an effective control structure for the system. Thus, as a starting point, the following two "original" configurations are presented:

1. Figure 2: This is the original configuration from the singular perturbation approach (Baldea and Daoutidis, 2006).
2. Figure 3: This is the simplest self-optimizing control configuration with control of the active constraints ($P_{reactor}$ and x_B) and self-optimizing variable W_S.

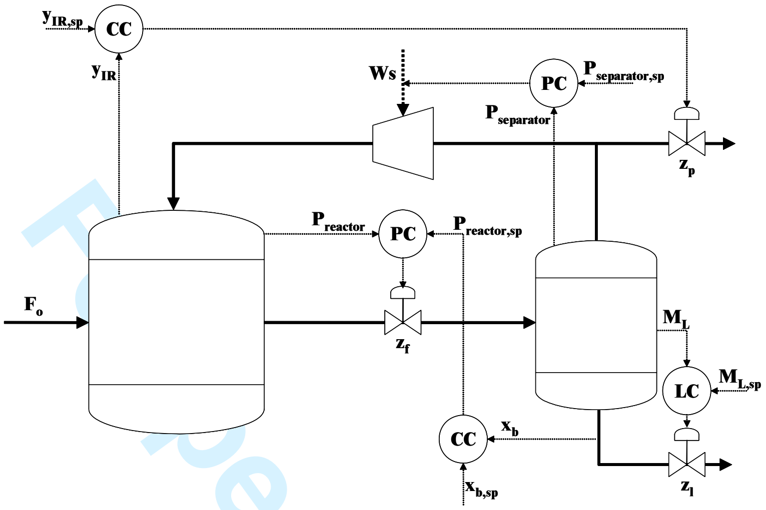

Fig. 2. Original configuration based on singular perturbation with control of x_B, $P_{separator}$, and $y_{I,R}$.

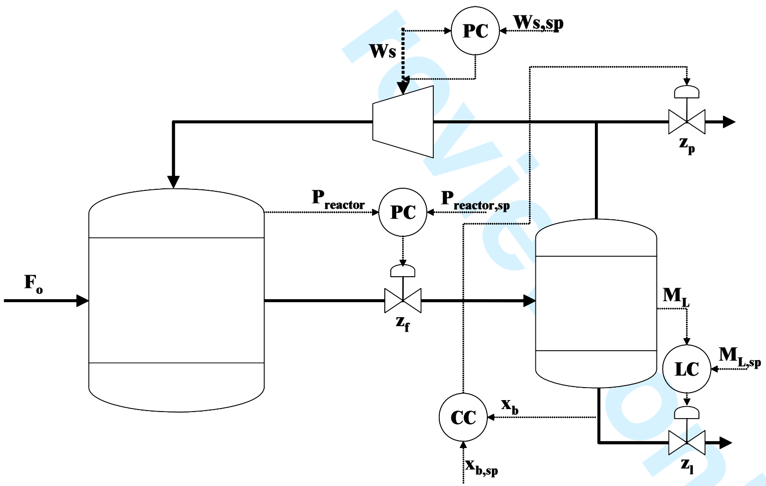

Fig. 3. Simplest self-optimizing configuration with control of x_B, $P_{reactor}$, and W_S.

None of these are acceptable. The configuration in Figure 2 is far from economically optimal and gives infeasible operation with the economic constraints $P_{reactor}$ exceeded. On the other hand, Figure 3 gives unacceptable dynamic performance. The idea is to combine the two approaches. Since one normally starts by designing the regulatory control system, the most natural is to start from Figure 2. The first evolution of this configuration is to change the pressure control from the separator to the reactor (Figure 4). In this case, both active constraints ($P_{reactor}$ and x_b) are controlled in addition to impurity level in the reactor ($y_{I,R}$). The final evolution is to change the primary controlled variable from $y_{I,R}$ to the compressor power W_s (Figure 5). The dynamic response for this configuration is very good and the economics are close to optimal.

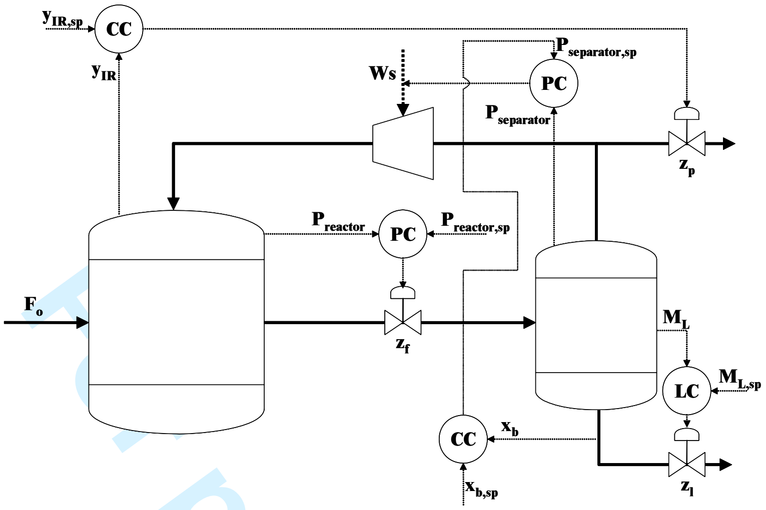

Fig. 4. Modification of Figure 2: Constant pressure in the reactor instead of in the separator.

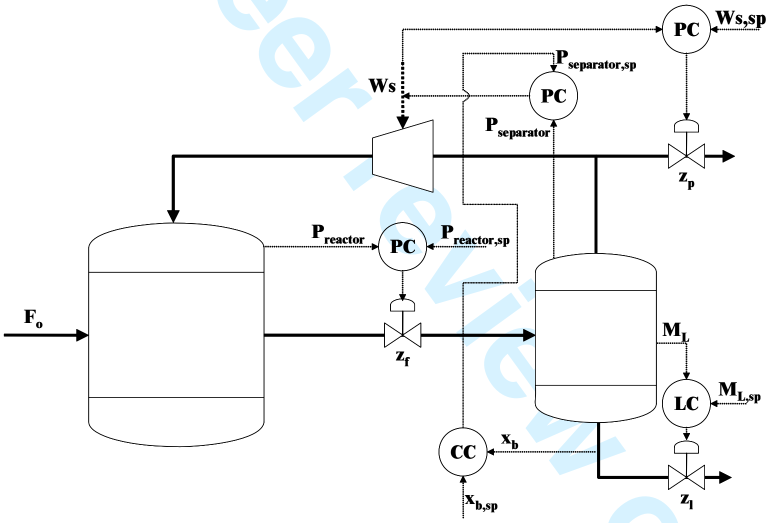

Fig. 5. Final structure from modification of Figure 4: Set recycle (W_S) constant instead of the inert composition ($y_{I,R}$).

4.4.1 Simulations

Simulations are carried out so the above configurations are assessed for controllability. Two major disturbances are considered: a sustained reduction of 10% in the feed flow rate F_o at $t = 0$ followed by a 5% increase in the setpoint for the product purity x_B at $t = 50$h. The results are found in Figures 6 through 9.

The original system in Figure 2 shows an infeasible response when it comes to increasing the setpoint of x_B since the reactor pressure increases out of bound (see

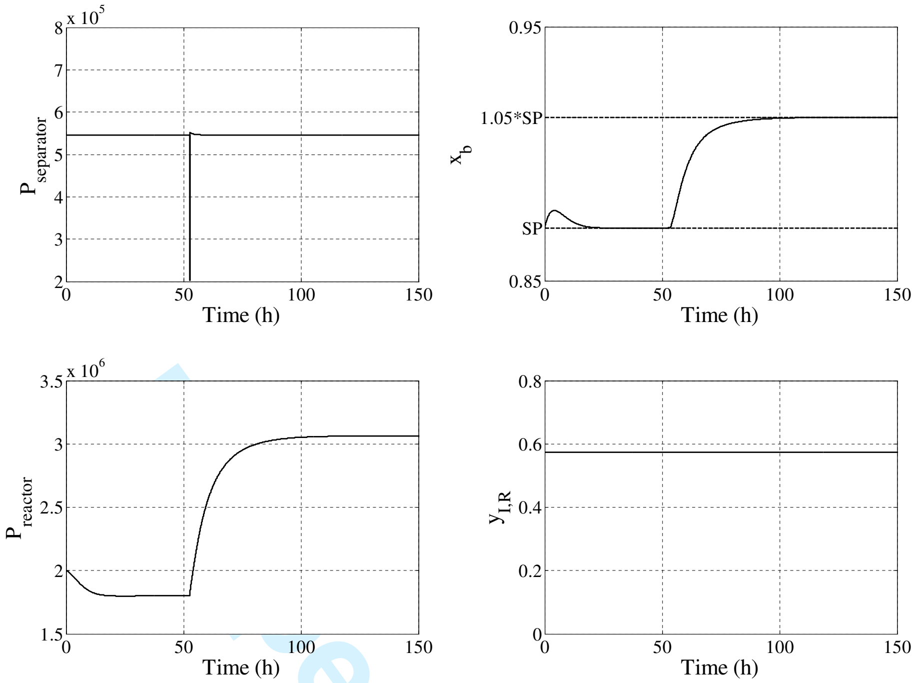

Fig. 6. Closed-loop responses for configuration in Figure 2: Profit = $43.13k\$/h$ and $43.32k\$/h$ (good but infeasible).

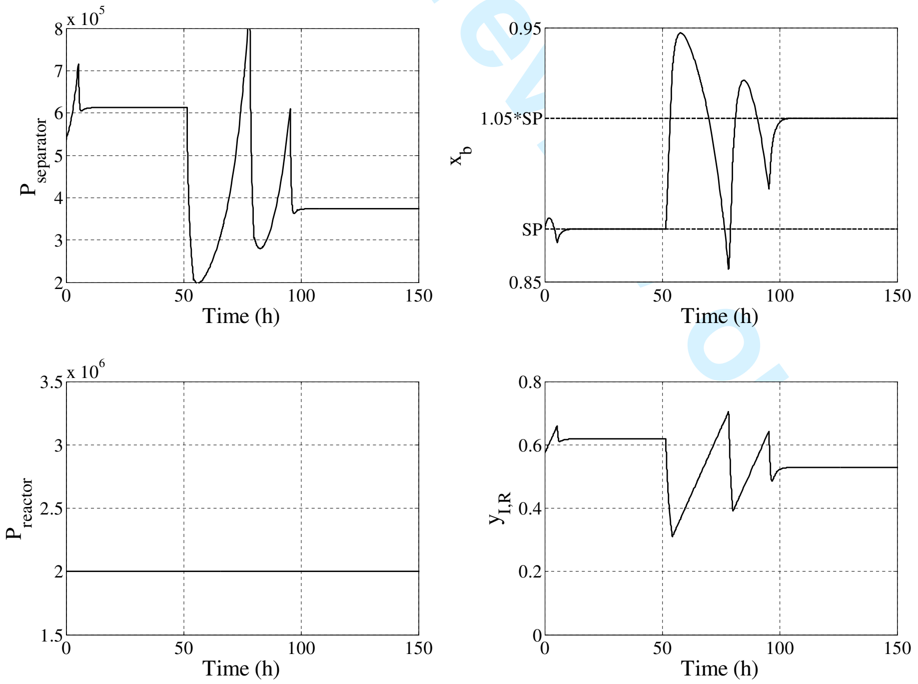

Fig. 7. Closed-loop responses for configuration in Figure 3: Profit = $43.21k\$/h$ and = $43.02k\$/h$.

Figure 6).

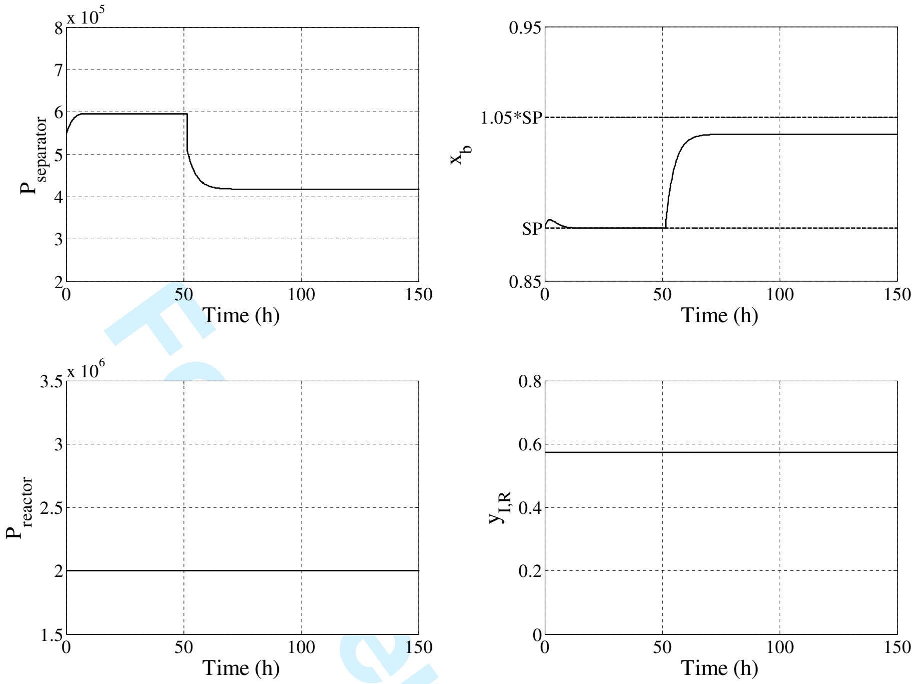

Fig. 8. Closed-loop responses for configuration in Figure 4: Profit = $43.20k\$/h$ and = $43.07k\$/h$.

With $P_{reactor}$ controlled (here integral action is brought about) by z_F (fast inner loop), the modified configuration shown in Figure 4 gives infeasible operation for setpoint change as depicted in Figure 8.

The proposed configuration in Figure 3, where the controlled variables are selected based on economics presents a very poor dynamic performance for setpoint changes in x_B as seen in Figure 7 due to the fact that the fast mode x_B is controlled by the small flow rate z_P and fast responses are obviously not expected, indeed the purge valve (z_P) stays closed during almost all the transient time.

Finally, the configuration in Figure 5 gives feasible operation with a very good transient behavior (see Figure 9).

In addition, the inert level, although not controlled in some of the proposed configurations, does not build up in the system even for long simulation times. Moreover, the liquid level in the separator is perfectly controlled for all configurations.

The steady-state profit for the two disturbances is shown in the caption of Figures 6 through 9.

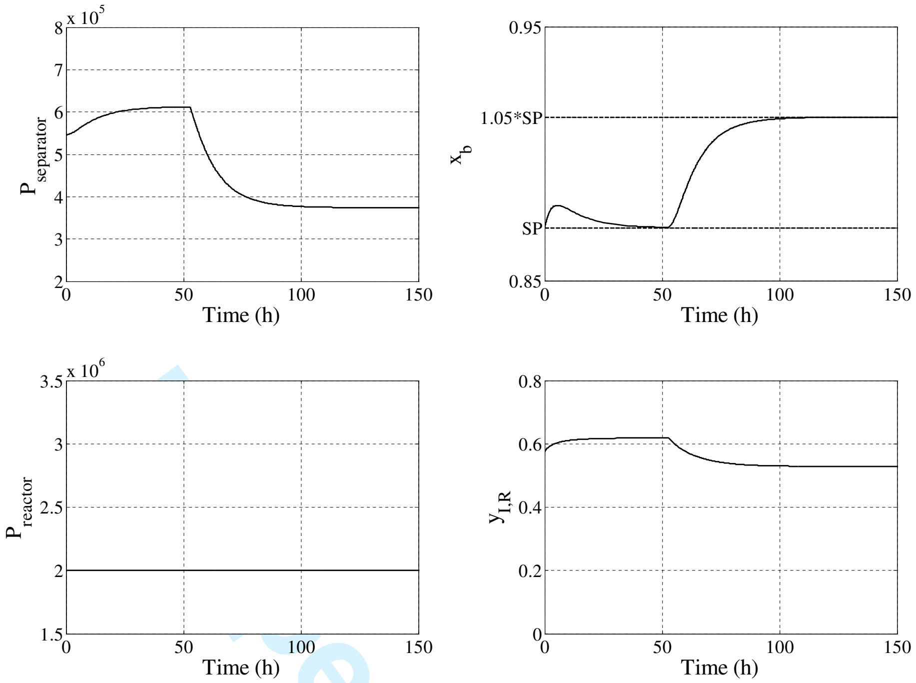

Fig. 9. Closed-loop responses for configuration in Figure 5: Profit = $43.21k\$/h$ and = $43.02k\$/h$.

5 Discussion

In the singular perturbation approach the model analysis may be used to tell which flows (inputs) are suitable for the different time scales. However, it can not be used to tell which outputs are needed to be controlled for economic reasons. Essentially, this approach sets the regulatory control layer in a hierarchical fashion, which represents a great advantage. In contrast, a plantwide control structure design cares for both supervisory and regulatory layers, where the self-optimizing control approach is used to set the former.

So, what is the link between these two approaches? The main link is that the singular perturbation approach can be used to "pair" the inputs (flows) with the outputs in the regulatory control layer resulting in a cascaded control configuration.

An economic analysis of the reactor-separator case study reveals the right variables to control in the slower control layer in order to keep the operation profitable (or at least near optimality). The reactor pressure, $P_{reactor}$ and product purity x_B are both active constraints that, during operation, must be kept constant at its setpoint together with the self-optimizing variable W_S.

In terms of speed of responses, the expectations are that:

1. Reactor pressure ($P_{reactor}$) is fast (in general, pressure requires fast control): prefer a large (gas) flow, i.e. F (z_F) or R (W_S). Particularly, one should use F (z_F) since R (W_S) is desired to be constant.
2. Separator liquid level (M_L) has intermediate speed: prefer using L (z_L) (intermediate flow).
3. Product purity (x_B) has also intermediate speed: it needs an intermediate flow, but since there are no such left since it is necessary to keep R (W_S) constant, one solution is to use R (W_S) dynamically for this (This is an interesting result that follows from the singular perturbation analysis!).
4. It is preferable to keep the compressor power (W_S) constant, but allowing it to vary dynamically as long as it is reset back to its desired value at steady state: the rule is to use the small purge flow P (z_P) for this.

6 Conclusion

This paper contrasted two different approaches for the selection of control configurations. The self-optimizing control approach is used to select the controlled outputs that gives the economically (near) optimal for the plant. These variables must be controlled in the upper or intermediate layers in the hierarchy. The fast layer (regulatory control layer) used to ensure stability and local disturbance rejection is then successfully designed (pair inputs with outputs) based on the singular perturbation framework proposed in Baldea and Daoutidis (2006). The case study on the reactor-separator network illustrates that the two approaches may be combined successfully.

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