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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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,

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

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 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.
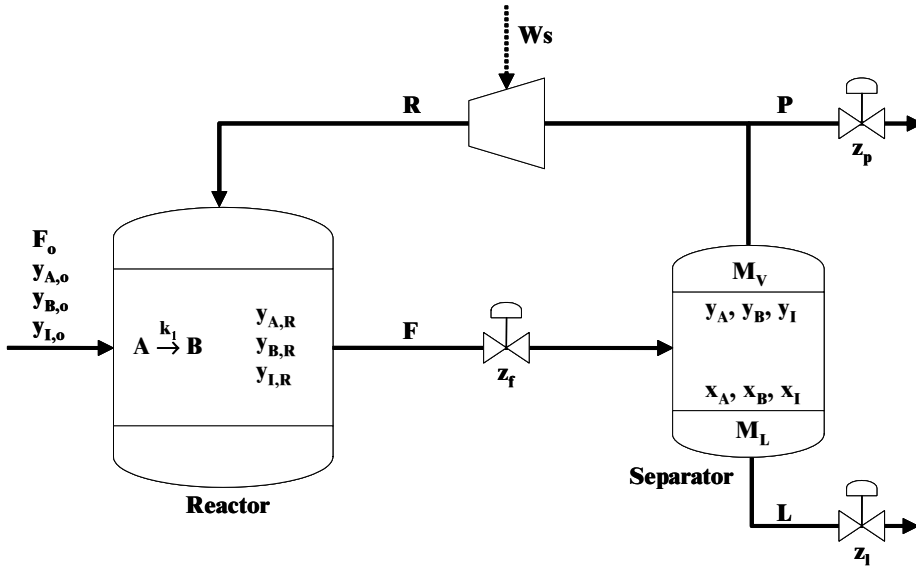

Fig. 1. Reactor-separator process.

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

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

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

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

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

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

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

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

$$N = N_A + N_B + N_I$$

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

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

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

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

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, 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.

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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:

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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.
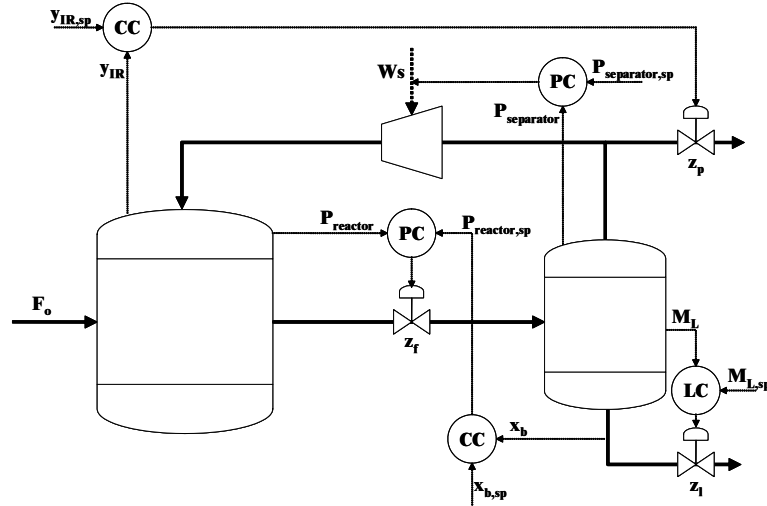

Fig. 2. Original configuration based on singular perturbation with control of x_B, $P_{separator}$, and $y_{I,R}$.
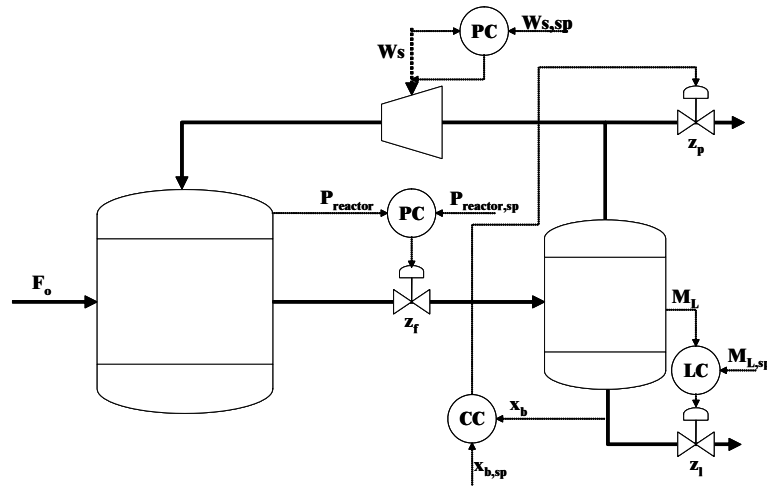

Fig. 3. Simplest self-optimizing configuration with control of x_B, $P_{reactor}$, and W_S.

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.
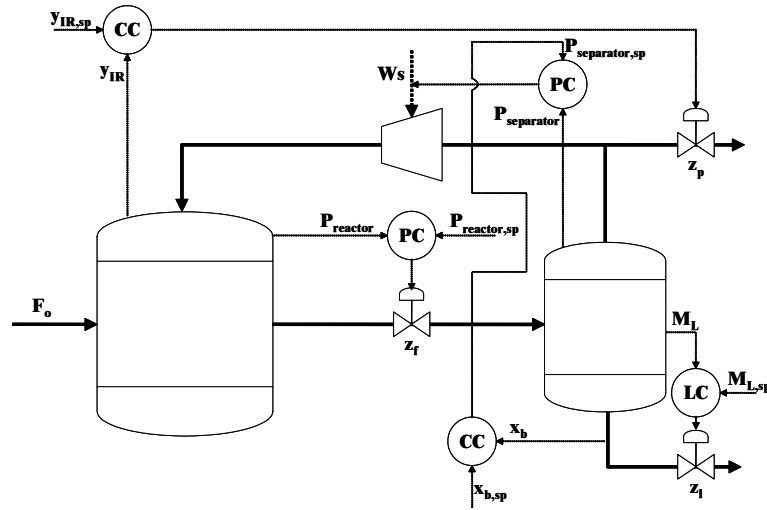

Fig. 4. Modification of Figure 2: Constant pressure in the reactor instead of in the separator.
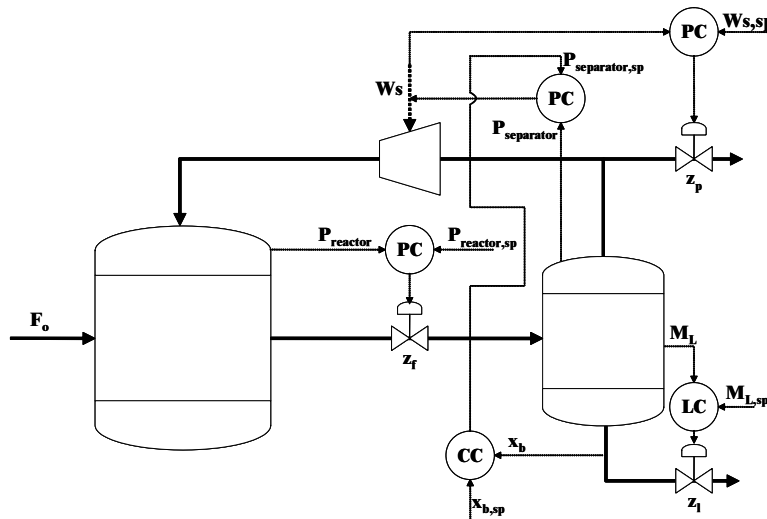

Fig. 5. Final structure from modification of Figure 4: Set recycle (W_S) constant instead of the inert composition ($y_{I,R}$).

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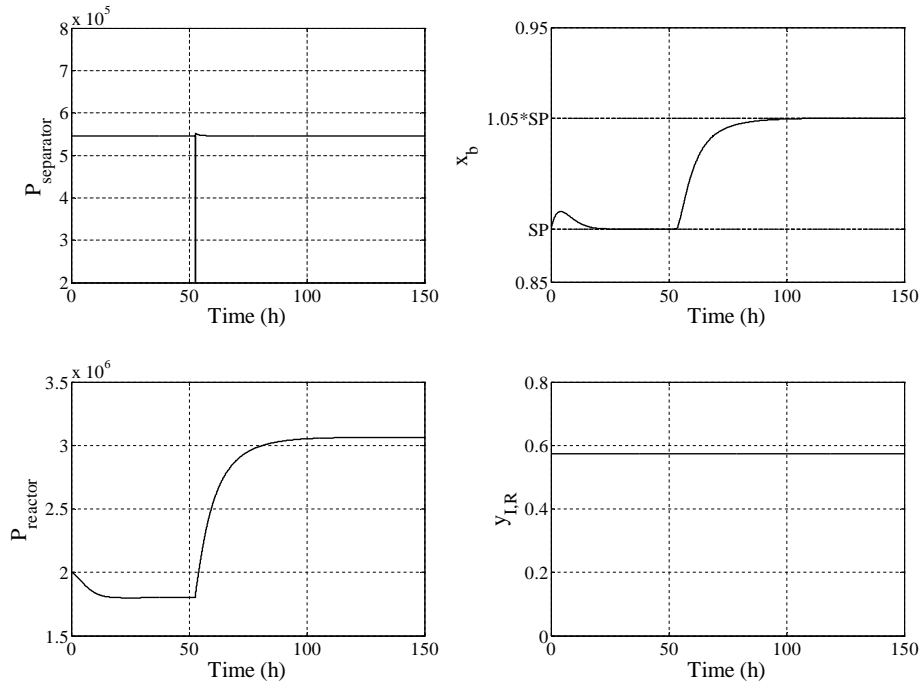
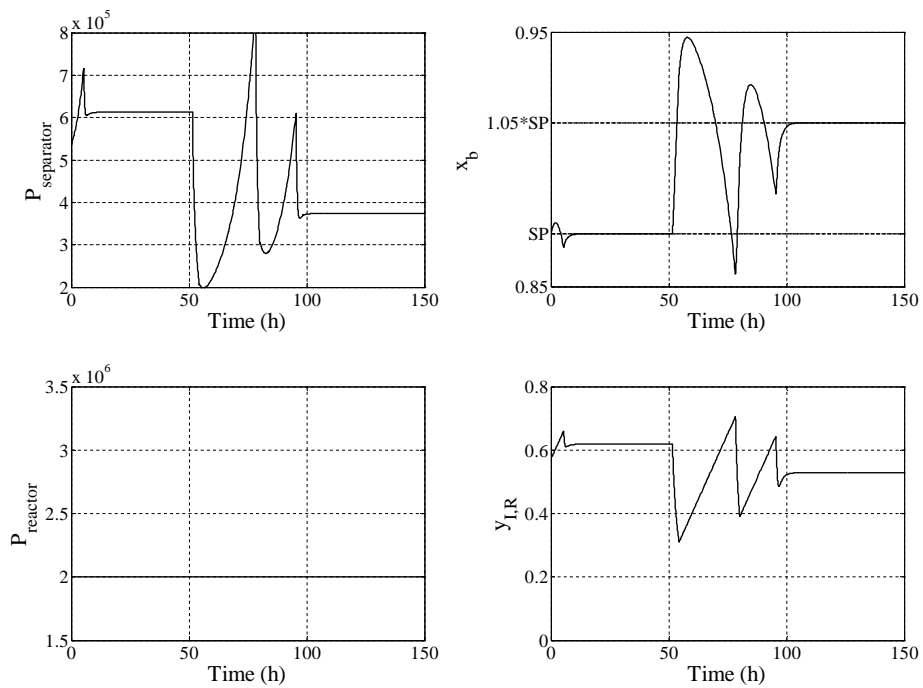Fig. 6. Closed-loop responses for configuration in Figure 2: Profit $= 43.13k\$/h$ and $43.32k\$/h$ (good but infeasible).

Fig. 7. Closed-loop responses for configuration in Figure 3: Profit $= 43.21k\$/h$ and $= 43.02k\$/h$.
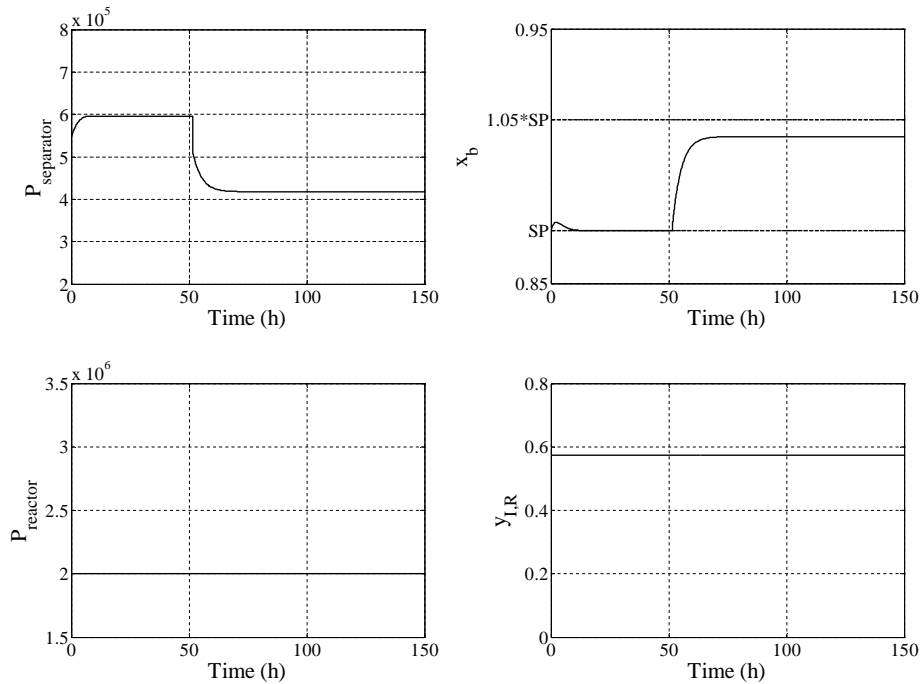
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Figure 6).

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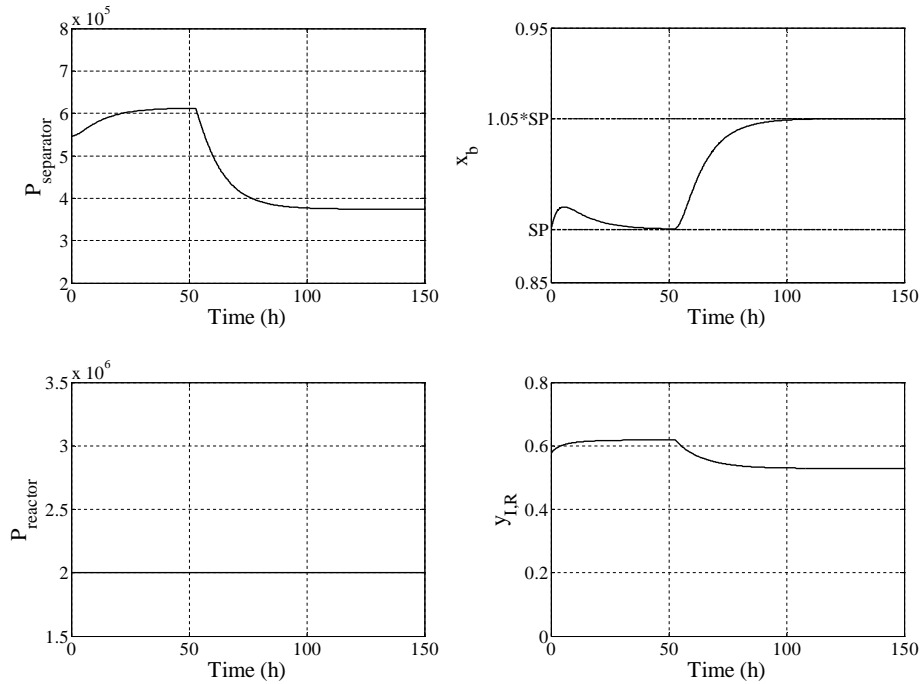
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Fig. 9. Closed-loop responses for configuration in Figure 5: Profit $= 43.21k\$/h$ and $= 43.02k\$/h$.

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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