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

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This paper aims at combining two different approaches ([1] and [2]) into a method for control structure design for plants with large recycle. The self-optimizing approach ([1]) 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 alternative is the singular perturbation framework proposed in [2] 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.

**Keywords:** 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., [2]) may warrant the use of multi-tiered control structures, and as 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,

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

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 have the best self-optimizing properties with the active constraints implemented.

## 3. TIME SCALE SEPARATION BY SINGULAR PERTURBATION ANALYSIS

In [2] and [3] 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.

## 4. CASE STUDY ON REACTOR-SEPARATOR 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 [3], but for the present paper the expressions for the flows $F$, $L$, $P$, and $R$ and economic data were added.

### 4.1. The reactor-separator 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 $x_B$.

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 $\rho_L$ 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.

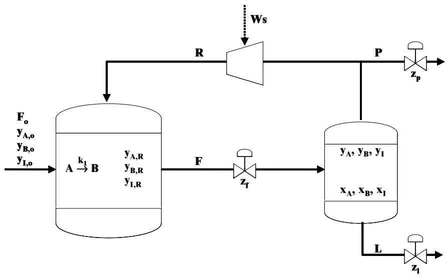


Figure 1. Reactor-separator process.

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

The open loop system has three 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.

The profit $(-J) = (p_L - p_P)L - p_W W_s$ is to be maximized 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.

The profit should be maximized subject to the following constraints: The reactor pressure $P_{reactor}$ should not exceed its nominal value and the product purity $x_b$ should be at least at its nominal value. In addition, there are bounds on the valve openings which must be within the interval [0 1] and the compressor power should not exceed its upper bound.

For optimization purposes the most important disturbances are the feed flow rate $F_o$, the feed compositions $y_{A,o}$, $y_{B,o}$ and $y_{I,o}$, the reaction rate $k_1$, and the reactor temperature $T_{reactor}$.

Two constraints are active at the optimal through all of 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 two degree of freedom since it is optimal to control them at their setpoint (active constraint control) leaving one unconstrained degree of freedom.

To find the remaining controlled variable, it is evaluated the loss imposed by keeping selected variables constant when disturbances occur and then picking the variable with the smallest *average* loss.

Accordingly, by the self-optimizing approach, the primary variables to be controlled are then $y = [P_{reactor}\ x_b\ W_s]$ with the manipulations $u = [z_f\ z_p\ W_s]$.

### 4.3. 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: $M_R$ ($P_{reactor}$) $\leftrightarrow$ $F$ ($z_f$); $M_V$ ($P_{separator}$) $\leftrightarrow$ $R$ ($z_p$); $M_L \leftrightarrow L$ ($z_l$); $x_b \leftrightarrow M_{R,setpoint}$ ($P_{reactor,setpoint}$); $y_{I,R} \leftrightarrow P$. It is important to note that no constraints are imposed in the variables in contrast to the self-optimizing control approach.

### 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 ([2]) from the singular perturbation approach.

**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 $W_s$.

Table 1
Dynamic model of the reactor-separator network.

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

$M_R$, $M_V$, and $M_L$ denote the molar holdups in the reactor and separator vapor and liquid phase, 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; $\epsilon$ the compressor efficiency; and $P_{reactor,max}$ is the maximum allowed pressure in the reactor.

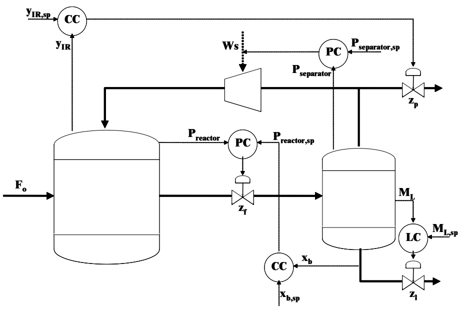


Figure 2. Original configuration based on singular perturbation with control of $x_b$, $P_{separator}$, and $y_{I,R}$.

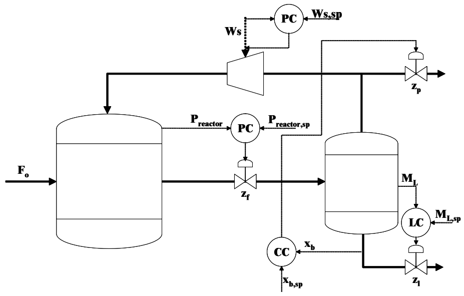


Figure 3. Simplest self-optimizing configuration with control of $x_b$, $P_{reactor}$, and $W_s$.

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.

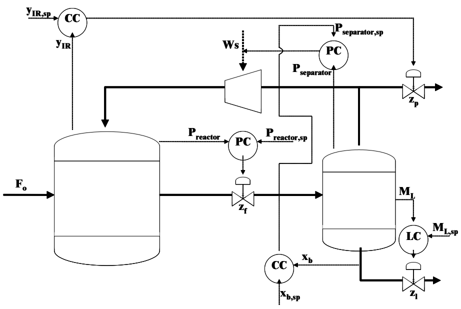


Figure 4. Modification of Figure 2: Constant pressure in the reactor instead of in the separator.

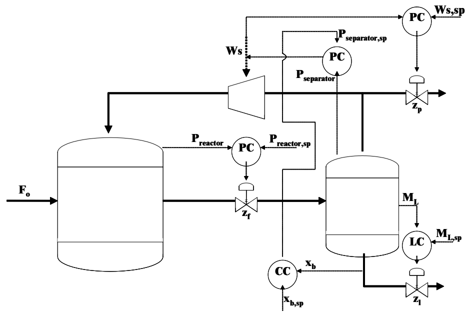


Figure 5. Final structure from modification of Figure 4: Set recycle ($W_s$) constant instead of the inert composition ($y_{I,R}$).

### 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.

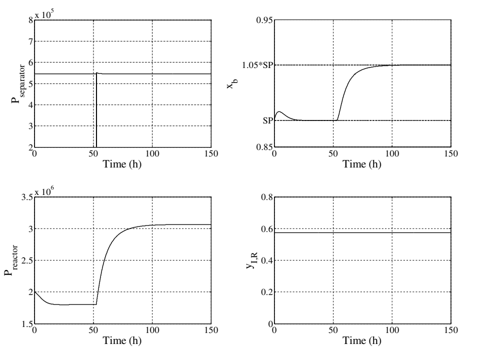


Figure 6. Closed-loop responses for configuration in Figure 2: Profit = $43.13k\$/h$ and $43.32k\$/h$ (good but infeasible).

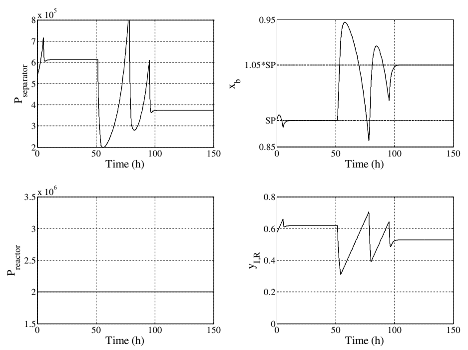


Figure 7. Closed-loop responses for configuration in Figure 3: Profit = $43.21k\$/h$ and = $43.02k\$/h$.

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 Figure 6).

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.

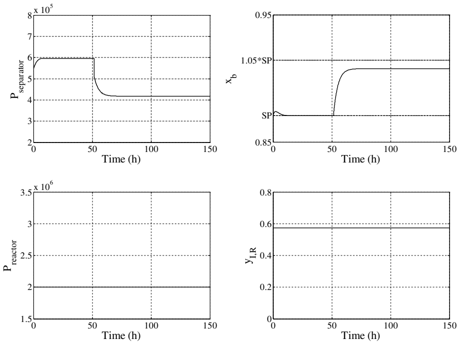


Figure 8. Closed-loop responses for configuration in Figure 4: Profit = $43.20k\$/h$ and = $43.07k\$/h$.

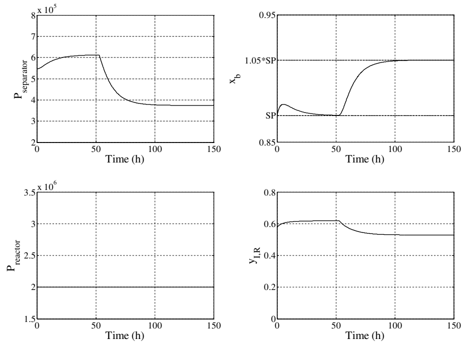


Figure 9. Closed-loop responses for configuration in Figure 5: Profit = $43.21k\$/h$ and = $43.02k\$/h$.

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).

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

## 5. 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 appropriately designed (pair inputs with outputs) based on a singular perturbation framework proposed in [2]. The case study on the reactor-separator network illustrates that the two approaches may be successfully combined.

## REFERENCES

[1] S. Skogestad. Plantwide control: The search for the self-optimizing control structure. *Journal of Process Control*, 10:487–507, 2000.

[2] M. Baldea and P. Daoutidis. Control of integrated process networks - a multi-time scale perspective. *Computers and Chemical Engineering. Submitted*, 2005.

[3] A. Kumar and P. Daoutidis. Nonlinear dynamics and control of process systems with recycle. *Journal of Process Control*, 12(4):475–484, 2002.