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Control of Integrated Process Networks – A Multi-Time Scale Perspective

M. Baldea [a] and P. Daoutidis [a,*]

[a] Department of Chemical Engineering and Materials Science, University of Minnesota, 421 Washington Ave. SE, Minneapolis, MN 55455, USA

Abstract

In this paper, we analyze the dynamics of integrated process networks featuring *large* recycle streams and *small* purge streams. We consider a prototype network comprising of a reactor and a condenser, and, within the framework of singular perturbations, we establish that the dynamics of such a network exhibits three time scales. We describe a model reduction procedure which leads to an explicit nonlinear description of the dynamics in each time scale, and we outline a controller synthesis procedure that rigorously accounts for this time-scale multiplicity.

Keywords: model reduction, singular perturbations, plant-wide control

1. Introduction

Process integration, through material and energy recycle streams, represents the rule, rather than an exception, in the process industries. While offering significant economic benefits, tightly integrated process networks pose distinct challenges, as the feedback interactions among the process units, induced by the recycle, give rise to complex, overall *network* dynamics, in addition to the dynamics of the individual units. Yet, most studies on control of process networks with recycle streams (e.g. Luyben, 1993; Yi and Luyben, 1997) are within a multi-loop linear control framework. The strong coupling between the control loops in such an approach has been recognized as a major issue that must be addressed in a plant-wide control setting (Price and Georgakis, 1993; Luyben et. al., 1997; Ng and Stephanopoulos, 1998, Larsson and Skogestad, 2000; Skogestad 2004).

In our previous work (Kumar and Daoutidis, 2002), we considered process networks with large material recycle. Within the framework of singular perturbations, we established that the large recycle induces a time scale separation, with the dynamics of individual processes evolving in a fast time scale, and the dynamics of the overall network evolving in a slow time scale. We proposed a model reduction method for deriving nonlinear low-order models of the slow dynamics and a controller design framework comprising of properly coordinated fast and slow controllers. In (Baldea et.

* Author to whom correspondence should be addressed. Email: daoutidi@cems.umn.edu.
P. Daoutidis currently at Aristotle University of Thessaloniki, Thessaloniki, Greece

al., 2004), we focused on process networks with recycle, in which small quantities of inert components are present and a small purge stream is used for their removal. Adopting again a singular perturbation perspective, we established the presence of a slow, core dynamics associated with the presence of the inert and outlined a framework for rationally addressing the control of inert levels in the network.

In the present paper, we analyze the dynamics of integrated process networks featuring large recycle streams *and* inert components purged through a small stream. Specifically, we consider a prototype network comprising of a gas phase reactor and a separation system with a gas recycle stream. Within the framework of singular perturbations, we establish that such a network exhibits three time scales: the fastest time scale, in the order of magnitude of the time constants of the individual units, a fast one, in which the dynamics of the entire network evolves, and a slow time scale associated with the presence of the inert and the small purge flowrate. Furthermore, we describe a model reduction procedure which leads to an explicit nonlinear description of dynamics in each time scale and we outline a controller synthesis procedure that rigorously accounts for the time-scale multiplicity feature of such networks. Finally, we provide illustrative numerical simulation results.

2. Modeling of Process Networks with Recycle and Purge

We consider the network of Figure.1, consisting of a gas-phase reactor and a condenser.

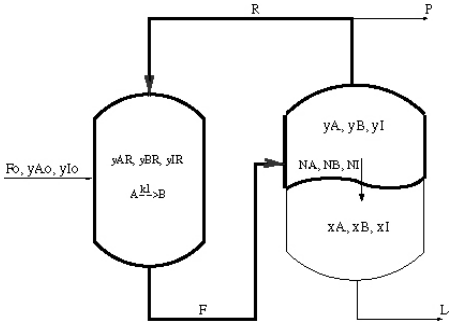

Figure 1. Process network with large recycle and purge

The reactant A is fed at a constant molar flowrate F_o to the reactor, where a first order, irreversible reaction takes place with reaction constant k_1. The outlet stream from the reactor is fed to a partial condenser that separates the light unconverted reactant *A* from the heavy product *B*. The gas phase is then recycled at a high rate back to the reactor. A very volatile impurity *I* is also present in the feed stream in small quantities, and a small purge stream *P* is used to remove this impurity from the recycle loop. The interphase mole transfer rates for the components *A*, *B*, *I* in the condenser are governed by rate expressions of the form $N_j = K_j\alpha(y_j - {}^{P_j^s}\!/_{P}\, x_j)\, {}^{M_L}\!/_{\rho_L}$, where $K_j\alpha$ represents a mass transfer coefficient, y_j the mole fraction in the gas phase, the mole fraction in the liquid phase, P^s_j the saturation vapour pressure of the component *j*, and *P* the pressure in the condenser. Assuming isothermal operation, the dynamic model of the network has the form:

$$
\begin{aligned}
&\dot{M}_R = F_o + R - F \\
&\dot{y}_{A,R} = \frac{1}{M_R}\Big[F_o(y_{A,o} - y_{A,R}) + R(y_A - y_{A,R}) - k_1 M_R y_{A,R}\Big] \\
&\dot{y}_{I,R} = \frac{1}{M_R}\Big[F_o(y_{I,o} - y_{I,R}) + R(y_I - y_{I,R})\Big] \\
&\dot{M}_V = F - R - N - P \\
&\dot{y}_A = \frac{1}{M_V}\Big[F(y_{A,R} - y_A) - N_A + y_A N\Big] \\
&\dot{y}_I = \frac{1}{M_V}\Big[F(y_{I,R} - y_I) - N_I + y_I N\Big] \\
&\dot{M}_L = N - L \\
&\dot{x}_A = \frac{1}{M_L}\Big[N_A - x_A N\Big] \\
&\dot{x}_I = \frac{1}{M_L}\Big[N_I - x_I N\Big]
\end{aligned}
\tag{1}
$$

where M_R, M_V, M_L denote the molar holdups in the reactor and condenser vapour and liquid phase, respectively, and $N=N_A+N_B+N_I$. We consider F_{os} to be $O(1)$, and define $\varepsilon_1=F_{os}/R_s$ as the ratio of the steady state values of the feed and recycle flowrates. Note that, due to the assumption that the recycle flowrate is much higher than the throughput, $\varepsilon_1 \ll 1$. Also, we define $\varepsilon_2 = P_s / F_{os} \ll 1$ (under steady-state conditions, the purge flowrate is much smaller than the feed), the scaled (possibly manipulated) inputs $u_R=R/R_s$, $u_F=F/F_s$ and $u_P=P/P_s$ and the $O(1)$ ratio $k=F_s/R_s$. We assume that the mole fraction of the inert in the feed is very small, i.e. $y_{I,o} = \alpha_I \varepsilon$, where $\alpha_I = O(1)$, that the inert is very volatile, i.e. $P_I^S / P = \alpha_2 / \varepsilon$, with $\alpha_2 = O(1)$, and that its mass transfer rate is very small, i.e. $K_I \alpha = \alpha_1 \varepsilon^2$, $\alpha_1 = O(1)$, the latter two assumptions implying that a negligible amount of inert leaves the recycle loop and exits through the liquid stream at the bottom of the condenser. Based on the above assumptions, the model of the process network takes the form:

$$
\begin{aligned}
&\dot{M}_R = F_o + \frac{1}{\varepsilon_1} F_{os}(u_R - k u_F) \\
&\dot{y}_{A,R} = \frac{1}{M_R}\left[F_o(1 - \alpha_I \varepsilon_2 - y_{A,R}) - k_1 M_R y_{A,R} + \frac{1}{\varepsilon_1} F_{os} u_R (y_A - y_{A,R})\right] \\
&\dot{y}_{I,R} = \frac{1}{M_R}\left[F_o(\alpha_I \varepsilon_2 - y_{I,R}) + \frac{1}{\varepsilon_1} F_{os} u_R (y_I - y_{I,R})\right] \\
&\dot{M}_V = -N_A - N_B - (\alpha_1 \varepsilon_2^2 y_I + \alpha_1 \alpha_2 \varepsilon_2 x_I)\frac{M_L}{\rho_L} + \frac{1}{\varepsilon_1} F_{os}(k u_F - u_R) - \varepsilon_2 F_{os} u_P \\
&\dot{y}_A = \frac{1}{M_V}\left[\frac{1}{\varepsilon_1} F_{os} k u_F (y_{A,R} - y_A) - N_A + y_A(N_A + N_B) + y_A(\alpha_1 \varepsilon_2^2 y_I + \alpha_1 \alpha_2 \varepsilon_2 x_I)\frac{M_L}{\rho_L}\right] \\
&\dot{y}_I = \frac{1}{M_V}\left[\frac{1}{\varepsilon_1} F_{os} k u_F (y_{I,R} - y_I) - (\alpha_1 \varepsilon_2^2 y_I + \alpha_1 \alpha_2 \varepsilon_2 x_I)\frac{M_L}{\rho_L} + y_I(N_A + N_B) + y_I(\alpha_1 \varepsilon_2^2 y_I + \alpha_1 \alpha_2 \varepsilon_2 x_I)\frac{M_L}{\rho_L}\right] \\
&\dot{M}_L = N_A + N_B + (\alpha_1 \varepsilon_2^2 y_I + \alpha_1 \alpha_2 \varepsilon_2 x_I)\frac{M_L}{\rho_L} - L \\
&\dot{x}_A = \frac{1}{M_L}\left[N_A - x_A(N_A + N_B) - x_A(\alpha_1 \varepsilon_2^2 y_I + \alpha_1 \alpha_2 \varepsilon_2 x_I)\frac{M_L}{\rho_L}\right] \\
&\dot{x}_I = \frac{1}{M_L}\left[(\alpha_1 \varepsilon_2^2 y_I + \alpha_1 \alpha_2 \varepsilon_2 x_I)\frac{M_L}{\rho_L} - x_I(N_A + N_B) - x_I(\alpha_1 \varepsilon_2^2 y_I + \alpha_1 \alpha_2 \varepsilon_2 x_I)\frac{M_L}{\rho_L}\right]
\end{aligned}
\tag{2}
$$

Evidently, the above model contains terms of $O(1)$, $O(1/\varepsilon)$ and $O(\varepsilon)$, which suggest potentially a three time scale behaviour. In what follows, we document this feature within the framework of singular perturbations.

3. Model Reduction and Control

We begin by obtaining a description of the fastest dynamics of the network. To this end, we define the fastest, stretched time scale $\tau_1=t/\varepsilon_1$. In the limit $\varepsilon_1 \to 0$, corresponding to an infinitely large recycle flowrate, we obtain the following description of the network dynamics in this fastest time scale:

$$\begin{array}{lll} \frac{M_R}{d\tau_1} = F_{os}(u_R - ku_F) & \frac{y_{A,R}}{d\tau_1} = \frac{F_{os}}{M_R}u_R(y_A - y_{A,R}) & \frac{y_{I,R}}{d\tau_1} = \frac{F_{os}}{M_R}u_R(y_I - y_{I,R}) \\ \frac{M_V}{d\tau_1} = F_{os}(ku_F - u_R) & \frac{y_A}{d\tau_1} = \frac{F_{os}}{M_V}ku_F(y_{A,R} - y_A) & \frac{y_I}{d\tau_1} = \frac{F_{os}}{M_V}ku_F(y_{I,R} - y_I) \\ \frac{M_L}{d\tau_1} = 0 & \frac{x_A}{d\tau_1} = 0 & \frac{x_I}{d\tau_1} = 0 \end{array} \quad (3)$$

Note that not all the nontrivial algebraic equations that correspond to the equilibrium of the fastest dynamics are linearly independent. Specifically, the last three nontrivial equations can be expressed as functions of the first three. This implies that the steady-state condition associated to the fastest dynamics does not specify isolated equilibrium points, but rather a six-dimensional manifold in which a slower dynamics evolves Also, note that the control objectives in this time scale must be addressed using the large inputs u^l, as the inputs u^s and u^p have no effect on the fastest dynamics. Turning now to the dynamics on this equilibrium manifold, multiplying Eq. (1) by ε_1 and considering the limit $\varepsilon_1 \to 0$, the linearly independent constraints: $0 = u_R - ku_F$, $0 = u_R(y_A - y_{A,R})$, $0 = u_R(y_I - y_{I,R})$ are obtained, which must be satisfied in the fast time scale. In this limit, the terms which involve division of the above functions with the small parameter ε_1 become indeterminate. Let z_1 denote these finite, but unknown terms. Then the model of the dynamics after the fastest boundary layer becomes a Differential Algebraic Equation (DAE) system of nontrivial index (owing to the unspecified variables z_1). Setting the large flowrates u^l with appropriate feedback laws (in the prototype network considered, we use u_R=1-k_{uR}($M_{V,sp}$-M_V) and u_F=1-k_{uF}($M_{R,sp}$-M_R)), the algebraic variables z_1 can be computed after one differentiation of the algebraic constraints (Kumar and Daoutidis, 2002). Thus, the index of the DAE system is exactly two. Employing a coordinate change which involves the total material holdup of the recycle loop, and the holdups of the individual components in the recycle loop, i.e.

$$\begin{array}{l} \xi_1 = M_R + M_V, \xi_2 = M_R y_{A,R} + M_V y_A, \xi_3 = M_R y_{I,R} + M_V y_I, \xi_4 = M_L, \xi_5 = x_A, \\ \xi_6 = x_I, \eta_1 = u_R(x) + ku_F(x), \eta_2 = u_R(x)(y_A - y_{A,R}), \eta_3 = u_R(x)(y_I - y_{I,R}) \end{array} \quad (4)$$

the resulting underlying ODE model becomes:

$$\dot{\xi}_1 = F_0 - N_A - N_B - \varepsilon_2\tilde{N}_I - \varepsilon_2 F_{os}u_P$$

$$\begin{aligned} \dot{\xi}_2 = &-(\varepsilon_2 F_{os} k\ k_{uF}\xi_2\ u_P + k_1\ \xi_2\ k_{uF}\ M_{R,sp} - kF_o\ y_{A,o}\ \xi_1\ k_{uF} + k\ k_{uF}\ N_A\ \xi_1 - kk_1\xi_2 \\ &+ k_1\ \xi_2\ \xi_1\ k_{uR} - F_o\ y_{Ao}\ \xi_1\ k_{uR} + k_{uR}\ N_A\ \xi_1 + k_1\ \xi_2 - k_1\ \xi_2\ k_{uR}\ M_{V,sp} \\ &+ \xi_2\ k_{uR}\ \varepsilon_2\ u_P\ F_{os})/(\xi_1\ (k\ k_{uF} + k_{uR})) \end{aligned}$$

$$\dot{\xi}_3 = \varepsilon_2(-\xi_3\ u_P\ F_{os} - \tilde{N}_I\ \xi_1 + F_o\ \alpha_I\ \xi_1)/\xi_1$$

$$\begin{aligned}\dot{\xi}_4 &= N_A + N_B + \varepsilon_2 \tilde{N}_I - L \\ \dot{\xi}_5 &= N_A - \xi_5 (N_A + N_B + \varepsilon_2 \tilde{N}_I) \\ \dot{\xi}_6 &= \varepsilon_2 \tilde{N}_I - \xi_6 (N_A + N_B + \varepsilon_2 \tilde{N}_I)\end{aligned} \tag{5}$$

with $\tilde{N}_I = (\alpha_1 \varepsilon_2 \xi_3 / \xi_1 + \alpha_1 \alpha_2 \xi_6) \xi_4 / \rho_L$. Notice that the above model is still stiff, due to the presence of the small singular perturbation parameter ε_2. Repeating the model decomposition procedure followed above, we can derive separate representations for the fast and slow dynamics. Specifically, considering the limit $\varepsilon_2 \to 0$ (corresponding to the absence of the inert component from the feed and a zero purge flowrate) in a slow, compressed, time scale $\tau_2 = t\varepsilon_2$ we obtain the following description of the slow dynamics

$$\frac{\mathrm{d}\xi_3}{\mathrm{d}\tau_2} = (-\xi_3 \ u_P \ F_{os} + F_o \ \alpha_I \ \xi_1) / \xi_1 \tag{6}$$

The control objectives at the network level (such as product purity, control of total material holdup, etc) can be achieved in the fast time scale using the manipulated inputs u^s, as neither the large inputs u^l, nor the purge stream have any effect in this time scale. Similarly, the control of the inert levels in the network can only be accomplished in the slow time scale using the purge stream u^p.

4. Simulation Study

We carried out simulation studies on a specific process network of the type presented in Figure 1, with the parameter values and nominal steady state given in Table 1.

Table 1. Nominal process parameters

M_R, mol	4007.0	ρ_L, mol/ m^3	15000.0	K_A, mol/ m^2 min	1140.0
M_V, mol	2710.33	$y_{A,o}$	0.98	K_B, mol/ m^2 min	1200.0
M_L, mol	1069.82	$y_{I,o}$	0.020	K_I, mol/ m^2 min	$60.0 \cdot 10^{-6}$
F_o, mol/ min	100	P_A^s, Pa	$1.16 \cdot 10^5$	α, m^2/ m^3	17.5
R, mol/ min	1002.73	P_B^s, Pa	$1.67 \cdot 10^5$	k_{uF}	0.05
F, mol/ min	1102.73	P_I^s, Pa	$5.67 \cdot 10^7$	k_{uR}	0.01
P, mol/ min	2.28	V_V, m^3	3.0	k_{uL}	0.04
k_1, 1/ min	0.06	T_R, K	373.0	T_{cond}, K	273.0

Specifically, we controlled the liquid level in the condenser (and, thereby, the total holdup of the network) using the effluent flowrate and a proportional controller, $L = L_s(1 - k_L(M_{L,sp} - M_L))$. Subsequently, we designed an input-output linearizing feedback controller with integral action (Daoutidis and Kravaris, 1992) for the product purity $x_B = 1 - x_A - x_I$, using the reactor holdup setpoint $M_{R,sp}$ as a manipulated input and requesting the critically damped second order response $x_B + \beta_1 \frac{dx_B}{dt} + \beta_2 \frac{d^2 x_B}{dt^2} = x_{B,sp}$ with $\beta_1 = 60$ min, $\beta_2 = 900$ min^2. Finally, we employed the derived reduced-order model of the slow dynamics (Eq. 6) to design an input-output linearizing controller with integral action for the total inert holdup, requesting the first order response $\xi_3 + \gamma \, d\xi_3 / dt = \xi_{3,sp}$ with

$\gamma = 1200\,\text{min}$. Figure 2 shows the closed-loop behaviour of the process network for a step change in the product purity setpoint $x_{B,sp}$ and in the presence of unmeasured disturbances. Clearly, the proposed controller exhibits a very good setpoint tracking and disturbance rejection performance.

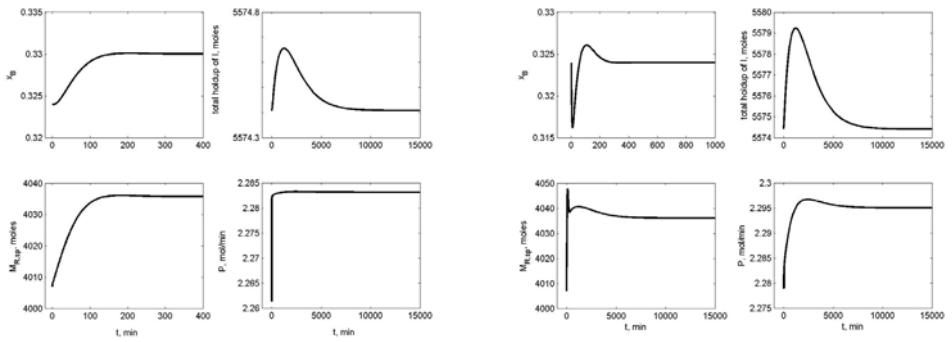

*Figure 2. Closed-loop responses of the reactor-condenser network for (**a**) a step change in the purity setpoint to 0.33 and (**b**) for a 20% estimation error of the mass transfer coefficient K_B*

5. Conclusions

In this paper, we analyzed the dynamic behaviour of integrated process networks with large recycle flows and small purge streams. Using a prototype network comprising of a reactor and a separator, we showed that such systems possess a dynamic behaviour featuring three distinct time scales and we outlined a controller design framework that naturally accounts for this time scale separation.

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