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Process Examples of Parallel Systems

APPENDIX I

Parallel process systems were introduced in Section 5.4, where a wide range of potential process behaviors were demonstrated. An important factor in determining the behavior for a specific system was shown to be the numerator, that is not a constant but contains the Laplace variable "s." Setting the numerator term (alone) to zero and solving for s provides a method for evaluating the numerator "zero." The possible step response behaviors are summarized below (for a stable system with real roots of the characteristic polynomial).

1. When the zero is negative and larger in magnitude than at least one pole, the dynamic step response of the output is an overdamped, S-shaped response.
2. When the zero is positive, the output experiences an inverse response.
3. When the zero is negative and smaller in magnitude than all poles, the output experiences an overshoot of its final value.

Importantly, overshoot requires unique controller design and tuning, and inverse response can be difficult to control for any feedback controller. Therefore, the engineer should understand how the process design and operation causes these unique dynamic behaviors. Two process examples are presented in detail in this appendix to provide a link between process technology and parallel systems.

EXAMPLE I.1. Heat exchanger with bypass.

Often a process stream must be heated or cooled a variable amount using a heat exchanger. A common method for variable heating is a heat exchanger with bypass, as shown in Figure I.1 for a cooler; the bypass provides the parallel struc-

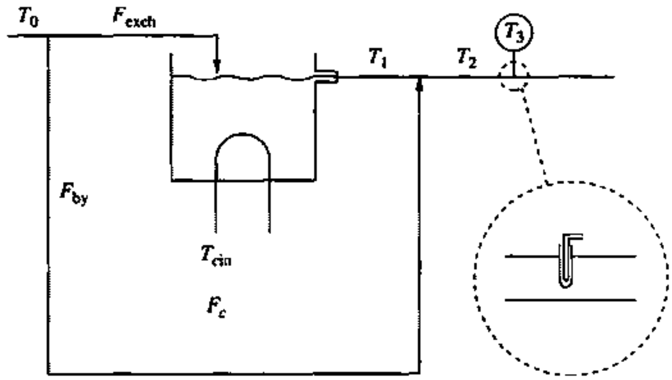

FIGURE I.1

Heat exchanger with bypass and sensor.

ture in this example. The flows through the exchanger and through the bypass are adjusted while the total process flow is maintained constant.

The behavior of an industrial shell-and-tube heat exchanger would be difficult to model, because it is a distributed-parameter system with complex flow patterns; therefore, the system is approximated as a stirred-tank heat exchanger, which retains the key properties of the system dynamics, in particular the response of the measured temperature signal to a step change in the flow to the exchanger.

Assumptions.

1. The same assumptions apply as in Example 3.7.
2. There is no transportation delay in short pipes.
3. The total flow (exchanger and bypass) is constant: $F_T = F_{exch} + F_{by} =$ constant.

Data. Note that these parameters are not realistic for a shell-and-tube heat exchanger, although the dynamic response is reasonable because the increased fluid inventory takes the place of the substantial metal capacitance.

1. $T_0 = 100°C$; $\rho = 10^6$ g/m^3; $C_p = 1$ cal/(g °C); $UA = 50 \times 10^6$ cal/(min °C); $T_{cin} = 60°C$; $\tau_3 = 0.5$ min; $V = 200$ m^3.
2. Initial steady state: $F_{by} = 50$ m^3/min; $F_{exch} = 50$ m^3/min; $T_1 = 80°C$; $T_2 = T_3 = 90°C$.
3. Input change: $\Delta F_{exch} = -10$ m^3/min at $t = 10$ min; consequently, $\Delta F_{by} = +10$ m^3/min.

Formulations. The fundamental model of the heat exchanger is the same as presented in Example 3.7, except that the feed flow rate, not the cooling medium flow, is changed in this example. Thus, model equations for the heat exchanger, bypass, and mixing are

$$\frac{dT_1}{dt} = \frac{F_{exch}}{V}(T_0 - T_1) - \frac{UA}{V\rho C_p}(T_1 - T_{cin}) \tag{I.1}$$

$$T_2 = \frac{F_{exch}T_1 + F_{by}T_0}{F_{exch} + F_{by}} = \frac{F_{exch}T_1 + (F_T - F_{exch})T_0}{F_T} \tag{I.2}$$

The temperature-measuring device is normally protected from contact with the process fluid by a metal sleeve called a *thermowell*, which introduces additional dynamic lag due to heat transfer dynamics associated with the thermowell. In this example, the thermowell dynamics are assumed to be well modelled by a first-order system with a time constant, τ_s, of 0.50 minutes (which is slower than most commercial sensor systems).

$$\tau_s \frac{dT_3}{dt} = T_2 - T_3 \tag{I.3}$$

with T_3 the signal from the sensor. These equations can be linearized, expressed in deviation variables, and transformed to the Laplace domain to give the individual transfer functions.

$$G_{ex} = \frac{T_1(s)}{F_{exch}(s)} = \frac{K_{exch}}{\tau_{exch}s + 1} \tag{I.4}$$

where
$$K_{exch} = \frac{(T_0 - T_1)_s \rho C_p}{(F_{exch})_s \rho C_p + UA} = 0.20 \frac{°\text{C}}{\text{m}^3/\text{min}}$$

$$\tau_{exch} = \frac{V \rho C_p}{(F_{exch})_s \rho C_p + UA} = 2.0 \text{ min}$$

$$G_{FM}(s) = \frac{T_2(s)}{F_{exch}(s)} = \frac{(T_1 - T_0)_s}{(F_{exch} + F_{by})_s} = K_{FM} = -0.20 \frac{°\text{C}}{\text{m}^3/\text{min}} \tag{I.5}$$

$$G_{TM}(s) = \frac{T_2(s)}{T_1(s)} = \frac{(F_{exch})_s}{(F_{exch} + F_{by})_s} = K_{TM} = 0.50 \frac{\text{m}^3/\text{min}}{\text{m}^3/\text{min}} \tag{I.6}$$

$$G_s(s) = \frac{T_3(s)}{T_2(s)} = \frac{1.0}{\tau_s s + 1} = \frac{1.0}{0.5s + 1} \tag{I.7}$$

The block diagram for this model is shown in Figure I.2, in which the parallel path is clearly evident, since the variable $F_{exch}(s)$ influences $T_2(s)$ through two paths. Note that for a parallel path to exist, a split must occur in the block diagram. The overall transfer function, relating the flow to the exchanger to the measured temperature, can be derived from block diagram algebra.

$$T_3(s) = G_s(s)[G_{FM}(s) + G_{TM}(s)G_{ex}(s)]F_{exch}(s) \tag{I.8}$$

$$\frac{T_3(s)}{F_{exch}(s)} = \frac{K_{FM}}{\tau_s s + 1} + \frac{K_{exch}K_{TM}}{(\tau_{exch}s + 1)(\tau_s s + 1)}$$
$$= \frac{(K_{FM} + K_{exch}K_{TM})\left[\left(\frac{K_{FM}\tau_{exch}}{K_{FM} + K_{exch}K_{TM}}\right)s + 1\right]}{(\tau_{exch}s + 1)(\tau_s s + 1)} = \frac{-0.1(4s + 1)}{(2s + 1)(0.5s + 1)} \tag{I.9}$$

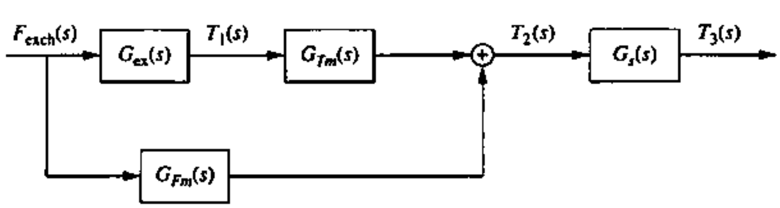

FIGURE I.2

Block diagram of exchanger with bypass and sensor.

From equation (I.9) we conclude that the poles of the overall system are the [illegible] of the individual systems. In this example the system is second-order with [illegible] distinct poles at $-1/\tau_{exch}$ and $-1/\tau_s$; thus, it is stable and is not periodic.

Due to the parallel structure, the transfer function has a zero in the numerator, which for this example is at $s = -(K_{FM} + K_{exch}K_{TM})/K_{FM}\tau_{exch}$ and is real and negative for this example. This zero can significantly affect the dynamic behavior of the system; therefore, the response of the system to a step input cannot be determined using Figure 5.5, which assumed a constant numerator. The dynamic response can be determined by inverting the Laplace transform of $T_3(s)$ for a step in $F_{exch}(s)$.

Solution. By substituting the data in the problem statement into equation (I.9), including the step input, $F_{exch}(s) = -10/s$, and determining the inverse using entry 10 in Table 4.1, the following analytical solution for the linear approximation can be found:

$$T_3'(t) = 1.0 - 2.333e^{-t/0.5} + 1.333e^{-t/2} \tag{I.10}$$

Results analysis. Dynamic responses are given in Figure I.3 for the nonlinear and approximate linearized models. They both show that the system output, T_3, overshoots and then approaches its final value smoothly. (The occurrence of the overshoot depends on the relative magnitudes of the numerator and denominator time constants.) The time at which the maximum occurs can be determined by setting the derivative of equation (I.10) to zero and solving for time, giving $t = 1.3$ minutes after the step. Thus, the parallel structure has fundamentally altered the dynamic behavior of this second-order system.

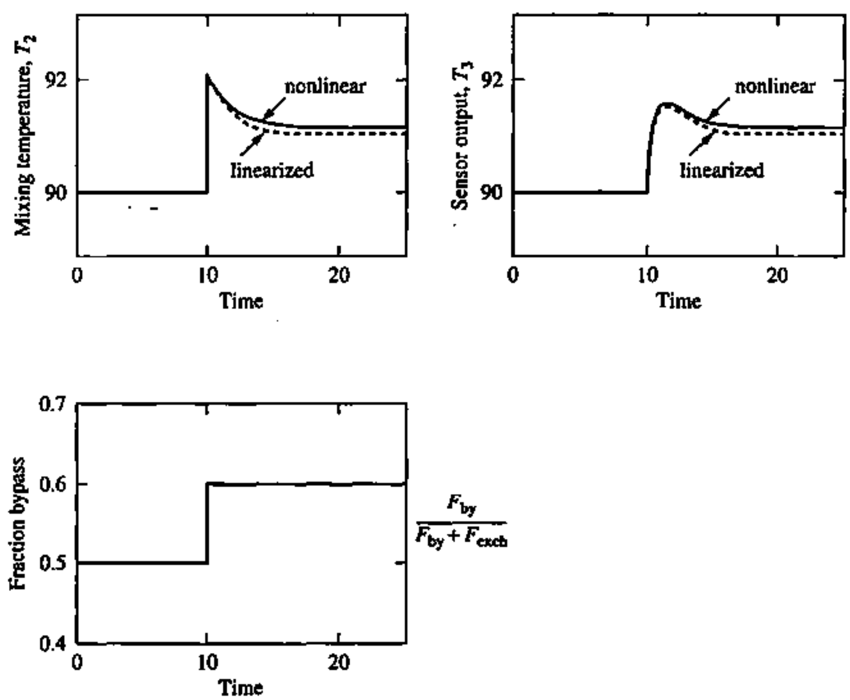

FIGURE I.3

Nonlinear and linearized dynamic responses for Example I.1.

The reason for this behavior can be understood by considering the two parallel paths in the physical system. When the exchanger flow is decreased, temperature T_1 is initially unaffected, and the modified flow ratio to the mixing point results in an immediate increase in temperature T_2. However, the exchanger outlet temperature T_1 decreases with a first-order response because of the lower flow to the exchanger. As a result, the mixture temperature decreases from its initial peak to its final value with a first-order response. The measured temperature follows the mixture temperature after the sensor first-order lag. Note that the overshoot is not due to a complex pole and that the behavior is *not periodic*. Rather,

> The unique behavior is due to parallel process paths with significant differences in dynamics for the two paths.

Naturally, such behavior should be considered in designing and operating the process. Imagine driving an automobile that tends to overshoot the change in direction indicated by the steering wheel; a careful and skilled driver (or control algorithm) would be required.

EXAMPLE I.2. Series reactors.

This example demonstrates that the parallel paths do not have to be external bypass streams but can be separate mechanisms within a single process. The process considered is a series of two CSTRs, shown in Figure I.4, with the same vessel size, flow rate, and chemical reaction as in Example 3.3; thus, the reactor models are identical to those derived in Example 3.3, equations (3.24) and (3.25) (page 64). In this example the response of the reactant concentration at the outlet of the second reactor to a step change in the solvent flow is to be determined.

Formulation. In this example the flows of the reactant and solvent can be changed independently. Also, the solvent flow is so much larger than the component A flow (F_A) that we assume that the total flow is the solvent flow; that is, $F \approx F_s$ and $C_{A0} \approx (C_A F_A)/F_s$. (Note that $F_s = 0.085$ and $C_{A0} = 0.925$, so that $C_A F_A = 0.0786$ mole/min.) With these assumptions, the following transfer functions

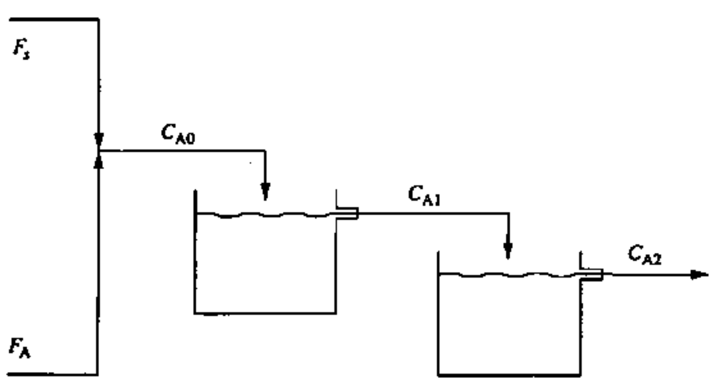

FIGURE I.4

Series chemical reactors for Example I.2.

can be derived:

$$\frac{C_{A0}(s)}{F_s(s)} = G_{mix}(s) = -\frac{C_A F_A}{(F_s)^2} = K_{mix} = -10.9 \ \frac{\text{mole/m}^3}{\text{m}^3/\text{min}} \tag{I.11}$$

$$\frac{C_{Ai}(s)}{F_s(s)} = G_{Fi}(s) = \frac{\dfrac{[C_{Ai-1}(s) - C_{Ai}(s)]_s}{F_s + Vk}}{\left(\dfrac{V}{F_s + Vk}\right)s + 1} = \frac{K_{Fi}}{\tau s + 1}$$

$$G_{F1}(s) = \frac{2.41}{8.25s + 1} \qquad G_{F2}(s) = \frac{1.61}{8.25s + 1} \tag{I.12}$$

$$\frac{C_{Ai}(s)}{C_{Ai-1}(s)} = G_{Ai}(s) = \frac{\dfrac{F_s}{F_s + Vk}}{\left(\dfrac{V}{F_s + Vk}\right)s + 1} = \frac{K_{Ai}}{\tau s + 1} = \frac{0.669}{8.25s + 1} \qquad \text{for } i = 1, 2 \tag{I.13}$$

The linearized model is represented in the block diagram in Figure I.5, which shows the parallel paths. In this example, the parallel paths result from the different effects of the solvent flow, through changes in the feed concentration and flow rate (residence time), on the outlet concentration of the second reactor. The overall transfer function can be derived using the block diagram to give the overall input-output relationship.

$$\frac{C_{A2}(s)}{F_s(s)} = G_{F2}(s) + G_{A2}(s)G_{F1}(s) + G_{A2}(s)G_{A1}(s)G_{mix}(s) \tag{I.14}$$

This expression clearly shows that three separate effects of the input influence the output concentration. The first effect, $G_{F2}(s)$, is of the flow or residence time in the second reactor; this effect begins instantaneously and increases the concentration. The second effect, $G_{A2}(s)G_{F1}(s)$, is the residence time in the first reactor, which increases the feed concentration to the inlet to the second reactor. The third effect involves the decrease in the feed concentration, C_{A0}; this effect is slower but of greater magnitude, ultimately decreasing the second reactor outlet concentration. The overall effect can be determined by substituting the individual transfer functions into equation (I.14) and rearranging to give

$$\begin{aligned} \frac{C_{A2}(s)}{F_s(s)} &= \frac{K_{F2}(\tau s + 1) + K_{A2}K_{F1} + K_{A2}K_{A1}K_{mix}}{(\tau s + 1)^2} \\ &= \frac{-1.66(-8.0s + 1)}{(8.25s + 1)^2} \end{aligned} \tag{I.15}$$

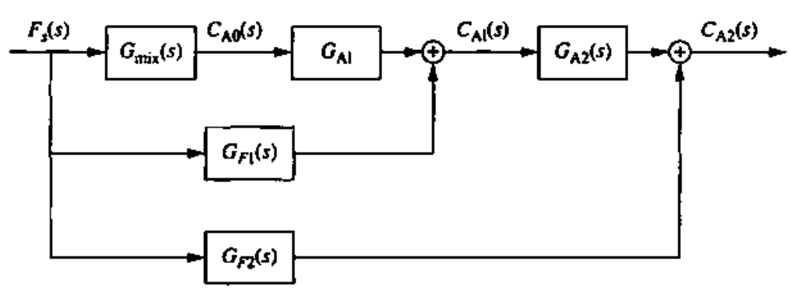

FIGURE I.5

Block diagram of reactors in Example I.2.

Again, the system is second-order and has the same poles as the individual elements in the system, but because of the numerator dynamics the response cannot be determined from a simple series system (i.e., Figure 5.5). Also, the result in this example is different from the previous example, because the transfer function in equation (I.15) has a *positive* numerator zero ($s = 1/8.0$). This is due to the last term in the numerator being large and negative, since K_{mix} is less than zero. This result indicates a mechanism for inverse response of the output variable, in which the initial response of the output can have the sign *opposite* to its final, steady-state change.

Solution. Again, the response can be determined by solving for the inverse Laplace transform using Table 4.1, entry 8. Substituting the data in the problem statement, including the input step of $F_S(s) = \Delta F_s/s = 0.0085/s$, gives

$$C_{A2}(t) = -0.0141 + (0.0141 + 0.00337t)e^{-t/8.25} \tag{I.16}$$

Results analysis. The response to a step change in the solvent feed flow, with reactant flow unchanged, is shown in Figure I.6 for the nonlinear and approximate linearized models. Note that the outlet reactant concentration initially *increases*, because of the decrease in residence time, which affects both reactors, including the last, immediately. However, the decreased feed concentration decreases the reactant concentration, initially in the first reactor and ultimately in the final reactor. Thus,

> The outlet concentration in the second reactor experiences an initial inverse response, because the fast effect of the residence time influences the output before the larger, slower feed concentration effect.

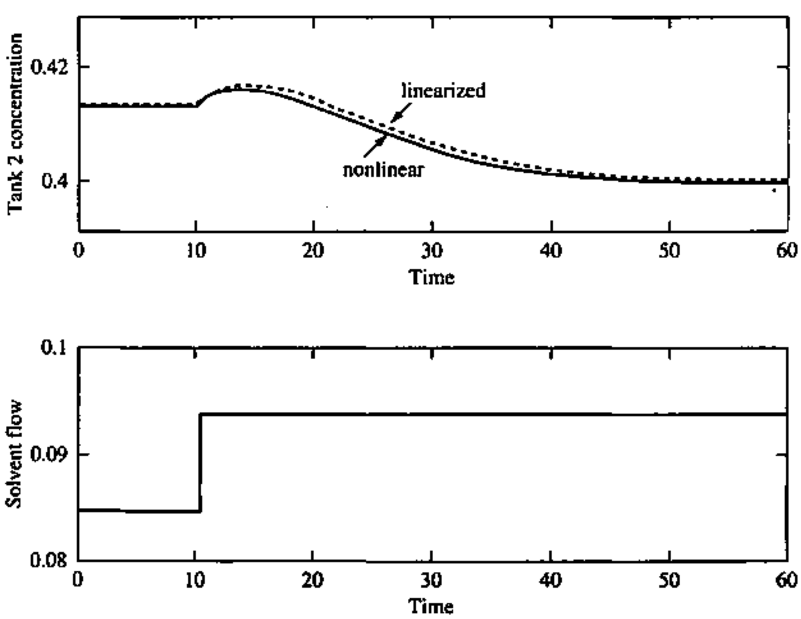

FIGURE I.6

Response for series chemical reactor to step in solvent flow in Example I.2.

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Behavior similar to this example is observed in other physical systems, especially tubular reactors. The series of CSTRs is selected in this example because the mathematical analysis is simpler, but lumped systems in series can serve as an approximation for the distributed system (Himmelblau and Bischoff, 1968). Modelling and experimental results for inverse responses in tubular reactors are presented by Silverstein and Shinnar (1982) and Ramaswamy et al. (1971).

The dynamic characteristics demonstrated in this example would be expected to have great influence on feedback control. Imagine driving an automobile that responded initially in the inverse direction to a change in steering! The most appropriate response would be to eliminate the inverse response by redesigning the process, if possible.

REFERENCES

Himmelblau, D., and K. Bischoff, *Process Analysis and Simulation: Deterministic Systems*, Wiley, New York, 1968.

Ramaswamy, V., F. Stermole, and K. McKinstry, "Transient Response of a Tubular Reactor to Upsets in Flow Rate," *AIChE J*, 17, 1, pp. 97–101 (1971).

Silverstein, J., and R. Shinnar, "Effect of Design on Stability and Control of Fixed Bed Catalytic Reactors with Heat Feedback. 1. Concepts," *IEC PDD, 21*, pp. 241–256 (1982).

QUESTIONS

I.1. Determine the response of the measured temperature T_3 to a step change in the coolant flow rate in the process in Figure I.1 and Example I.1. Based on the dynamics, would you prefer to manipulate the coolant flow rate or the bypass flow to control T_3?

I.2. Determine the response of the measured temperature T_3 to a step in the inlet temperature T_0. Discuss the similarities and differences of this behavior to the dynamic response in equation (I.9) and Figure I.3.

I.3. A model and dynamic response are derived in Example I.2 for a series of two chemical reactors. In the worked example, the solvent flow (F_s) is changed in a step and the outlet concentration experiences an inverse response. Determine the dynamic response for a step change of ΔF_A, with all other inputs constant. All assumptions are the same as in Example I.2, and you may use relevant results without deriving. The answer to this question should include an analytical expression for the response of C_{A2} and a description of the dynamic response of the concentration in the second reactor. Compare your results with Figure I.5, and discuss whether controlling C_{A2} would be easier or more difficult by manipulating F_A.

I.4. The series of two chemical reactors described in Example I.2 is the initial process upon which this question is based. You may use all results from the modelling in Example I.2 without proving, simply cite the source of the equations.

(*a*) The solvent flow and composition at the inlet to the first reactor are to be controlled by two single-loop controllers. By adding sensors and final elements as required, describe briefly and sketch a control system for this purpose.

(*b*) Given this strategy is functioning perfectly (maintaining C_{A0} *constant*), determine the model between the solvent flow and the concentration of the reactant in the second reactor, C_{A2}, and comment on the expected composition (C_{A2}) control performance using this manipulated-controlled variable pairing.

(*c*) Compare with the control performance in Example 13.8.

I.5. The dynamic response of a CSTR is considered in this question. You are to determine the characteristics of the response in component B in the effluent to a change in feed flow rate. You should determine the order, stability, damping, and effect of numerator zero from parallel paths. Based on your analysis, discuss whether a feedback controller from effluent concentration of B (C_B) to feed flow (F) would perform well.

Assumptions:

1) The reactor is well mixed and has a constant liquid volume.
2) The reactor is isothermal.
3) The density of the reactant and products are identical.
4) Only reactant (A) and solvent are present in the feed and the feed composition is constant.

Data:

1) The reaction is described by the following elementary reactions.

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

where $\quad -r_A = k_1 C_A$ and $-r_B = k_2 C_B$