Commande de procédés, Test May 2017

Surname:

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Problem 1 (Modeling) [2 points]

Consider a semi-batch reactor in which the reactions R1 (A+B→C+D) and R2 (2A+B→2C+E) take place. The inlet volumetric flowrate is equal to q. The inlet concentration of the chemical species A is denoted as $c_{A,e}$, whereas the inlet temperature is denoted as T_e. Moreover, c_A, c_B, c_C, c_D, c_E represent the concentrations of A, B, C, D and E in the reactor and T represents the temperature.

The reaction mixture has the volume V, and its density ρ and specific heat capacity c_p are constant. The reactor exchanges heat with its jacket, which is at a temperature T_j and is characterized by a heat transfer coefficient U (per unit of area) and an exchange area A. The enthalpies of reaction of R1 and R2 (per number of moles of product) are equal to ΔH_1 and ΔH_2.

The reaction rates of R1 and R2 (per unit of volume) are $k_1 c_A c_B$ and $k_2 c_A^2 c_B$. According to the Arrhenius' law, each rate constant k_i in a nonisothermal reactor is given by $A_i \exp\left(-\frac{E_i}{RT}\right)$, where A_i is the pre-exponential factor, E_i is the activation energy, and R is the ideal gas constant.

1. Write the dynamic model for this reactor using V, c_A, c_B and T (but not c_C, c_D nor c_E) as state variables.
2. What would be different in the dynamic model of a continuous stirred tank reactor with constant volume V and inlet and outlet volumetric flowrates q?

Solution:

1. First of all, from the mass balance

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho V) = \rho q,$$

one obtains

$$\dot{V} = q.$$

From the mole balance for A

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(c_A V\right) = q c_{A,e} + V\left(-A_1 \exp\left(-\tfrac{E_1}{RT}\right) c_A c_B - 2A_2 \exp\left(-\tfrac{E_2}{RT}\right) c_A^2 c_B\right),$$

one can obtain the dynamic equation for c_A:

$$\dot{c}_A = \frac{q}{V}\left(c_{A,e} - c_A\right) - A_1 \exp\left(-\tfrac{E_1}{RT}\right) c_A c_B - 2A_2 \exp\left(-\tfrac{E_2}{RT}\right) c_A^2 c_B.$$

A similar mole balance for B yields the following dynamic equation for c_B:

$$\dot{c}_B = -\frac{q}{V} c_B - A_1 \exp\left(-\tfrac{E_1}{RT}\right) c_A c_B - A_2 \exp\left(-\tfrac{E_2}{RT}\right) c_A^2 c_B.$$

Finally, from the heat balance

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(V \rho c_p T\right) &= q \rho c_p T_e + UA\left(T_j - T\right) \\ &\quad + V\left(-\Delta H_1 A_1 \exp\left(-\tfrac{E_1}{RT}\right) c_A c_B - \Delta H_2 A_2 \exp\left(-\tfrac{E_2}{RT}\right) c_A^2 c_B\right),\end{aligned}$$

it is possible to write the dynamic equation for T:

$$\begin{aligned}\dot{T} &= \frac{q}{V}\left(T_e - T\right) + \frac{UA}{V \rho c_p}\left(T_j - T\right) \\ &\quad + \frac{(-\Delta H_1) A_1 \exp\left(-\tfrac{E_1}{RT}\right) c_A c_B + (-\Delta H_2) A_2 \exp\left(-\tfrac{E_2}{RT}\right) c_A^2 c_B}{\rho c_p}.\end{aligned}$$

2. In the case of a continuous stirred tank reactor, the dynamic equations for c_A, c_B and T would be exactly the same, but the volume V would be constant, whereas in the case of the semi-batch reactor in point 1 the volume V also varies according to the dynamic equation $\dot{V} = q$.

Problem 2 (Linearization) [1 point]

Consider the following dynamic equations that describe the level in two tanks connected by a valve:

$$
\begin{aligned}
\dot{h}_1 &= q_1/A - a_1\sqrt{h_1} - a_{12}\sqrt{h_1 - h_2}, \\
\dot{h}_2 &= a_{12}\sqrt{h_1 - h_2} - a_2\sqrt{h_2},
\end{aligned}
$$

with the following numerical values: $A = 100$ cm^2, $a_1 = 0.10$ cm$^{0.5}$ s^{-1}, $a_{12} = 0.08$ cm$^{0.5}$ s^{-1}, $a_2 = 0.06$ cm$^{0.5}$ s^{-1}.

1. Calculate the values $\bar{h}_1$ and $\bar{h}_2$ at steady state, knowing that $\bar{q}_1 = 74$ cm^3 s^{-1}.
2. Linearize the system around the point calculated in point 1.

Solution:

1. At steady state, $\dot{h}_1 = \dot{h}_2 = 0$. If the constant values are replaced in the dynamic equations, the system of equations to be solved is

$$
\begin{cases} 0 = \bar{q}_1/A - a_1\sqrt{\bar{h}_1} - a_{12}\sqrt{\bar{h}_1 - \bar{h}_2} \\ 0 = a_{12}\sqrt{\bar{h}_1 - \bar{h}_2} - a_2\sqrt{\bar{h}_2} \end{cases} \Leftrightarrow \begin{cases} 74 = 10\sqrt{\bar{h}_1} + 8\sqrt{\bar{h}_1 - \bar{h}_2} = 10\sqrt{\bar{h}_1} + 8\sqrt{\frac{9}{25}\bar{h}_1} \\ \bar{h}_2 = \frac{16}{25}\bar{h}_1 \end{cases},
$$

whose solution is the following:

$$
\begin{cases} \bar{h}_1 = \left(\frac{74}{10+24/5}\right)^2 = \left(5\frac{74}{50+24}\right)^2 = 25 \\ \bar{h}_2 = \frac{16}{25}\bar{h}_1 \end{cases} \Rightarrow \begin{cases} \bar{h}_1 = 25 \text{ cm} \\ \bar{h}_2 = 16 \text{ cm} \end{cases}.
$$

2. In the dynamic model given above, the nonlinear terms that need to be linearized are $\sqrt{h_1}$, $\sqrt{h_1 - h_2}$ and $\sqrt{h_2}$. It is known that

$$
\begin{aligned}
&\left[\frac{\partial\left(\sqrt{h_1}\right)}{\partial h_1}\right]_{\bar{h}_1,\bar{h}_2,\bar{q}_1} = \frac{1}{2\sqrt{\bar{h}_1}}, \left[\frac{\partial\left(\sqrt{h_1 - h_2}\right)}{\partial h_1}\right]_{\bar{h}_1,\bar{h}_2,\bar{q}_1} = \frac{1}{2\sqrt{\bar{h}_1 - \bar{h}_2}}, \left[\frac{\partial\left(\sqrt{h_2}\right)}{\partial h_1}\right]_{\bar{h}_1,\bar{h}_2,\bar{q}_1} = 0, \\
&\left[\frac{\partial\left(\sqrt{h_1}\right)}{\partial h_2}\right]_{\bar{h}_1,\bar{h}_2,\bar{q}_1} = 0, \left[\frac{\partial\left(\sqrt{h_1 - h_2}\right)}{\partial h_2}\right]_{\bar{h}_1,\bar{h}_2,\bar{q}_1} = -\frac{1}{2\sqrt{\bar{h}_1 - \bar{h}_2}}, \left[\frac{\partial\left(\sqrt{h_2}\right)}{\partial h_2}\right]_{\bar{h}_1,\bar{h}_2,\bar{q}_1} = \frac{1}{2\sqrt{\bar{h}_2}}.
\end{aligned}
$$

Then, if the dynamic model is linearized and written in deviation variables, it becomes

$$
\begin{cases} \delta\dot{h}_1 = -\left(\frac{a_1}{2\sqrt{\bar{h}_1}} + \frac{a_{12}}{2\sqrt{\bar{h}_1 - \bar{h}_2}}\right)\delta h_1 + \frac{a_{12}}{2\sqrt{\bar{h}_1 - \bar{h}_2}}\delta h_2 + \frac{1}{A}\delta q_1 \\ \delta\dot{h}_2 = \frac{a_{12}}{2\sqrt{\bar{h}_1 - \bar{h}_2}}\delta h_1 - \left(\frac{a_{12}}{2\sqrt{\bar{h}_1 - \bar{h}_2}} + \frac{a_2}{2\sqrt{\bar{h}_2}}\right)\delta h_2 \end{cases}.
$$

Problem 3 (Laplace transform) [1 point]

Consider the following dynamic system:

$$\ddot{y}(t) + 5\dot{y}(t) + 4y(t) = u(t),$$

with the initial conditions $y(0) = 1$, $\dot{y}(0) = -4$ and the input $u(t) = e^{-t}$.

1. Compute $y(t)$ using the Laplace transform.
2. What is the static gain and the damping factor of this system?

Solution:

1. Applying the Laplace transform gives

$$s^2Y(s) - s + 4 + 5\,(sY(s) - 1) + 4Y(s) = U(s),$$

which implies that

$$Y(s) = \frac{1}{(s+1)(s+4)}U(s) + \frac{1}{s+4},$$

with the transfer function $G(s) = \frac{Y(s)}{U(s)} = \frac{1}{(s+1)(s+4)}$. Since $U(s) = \frac{1}{s+1}$,

$$Y(s) = \frac{1}{(s+1)^2(s+4)} + \frac{1}{s+4} = \frac{s^2+2s+2}{(s+1)^2(s+4)}.$$

By applying partial fraction decomposition, one obtains

$$Y(s) = \frac{A}{(s+1)} + \frac{B}{(s+1)^2} + \frac{C}{(s+4)},$$

where

$$A = \lim_{s\to-1} \frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{s^2+2s+2}{s+4}\right) = \lim_{s\to-1} \frac{(2s+2)(s+4) - (s^2+2s+2)}{(s+4)^2} = -1/9,$$

$$B = \lim_{s\to-1} \frac{s^2+2s+2}{s+4} = 1/3,$$

$$C = \lim_{s\to-4} \frac{s^2+2s+2}{(s+1)^2} = 10/9,$$

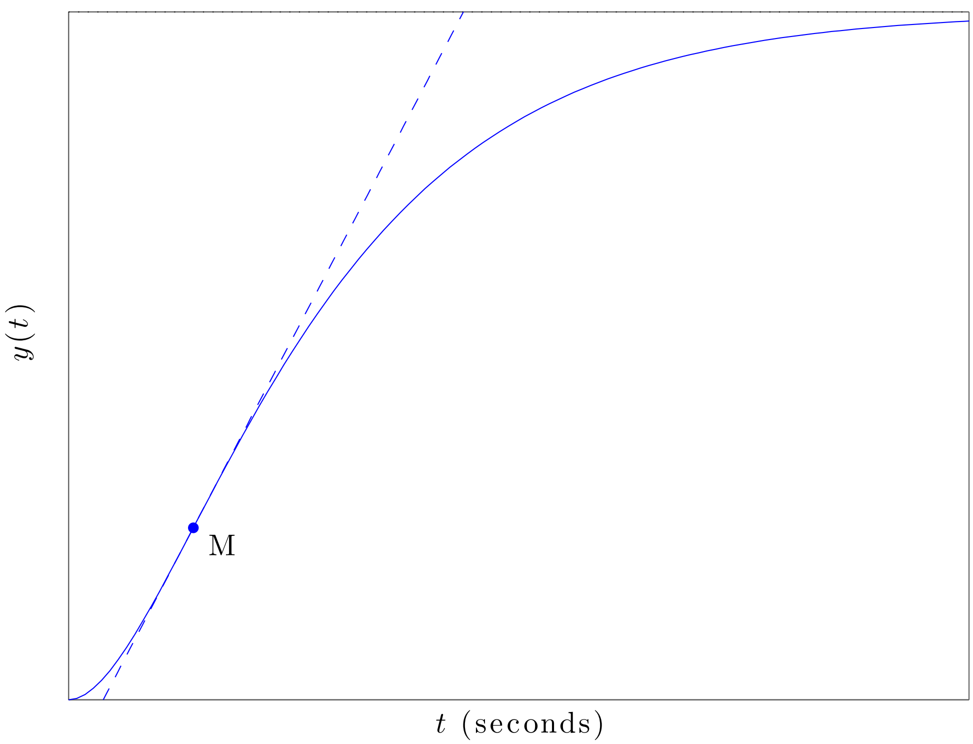
Taking inverse Laplace transformation gives

$$y(t) = \begin{cases} 0, & t < 0 \\ Ae^{-t} + Bte^{-t} + Ce^{-4t}, & t \geq 0 \end{cases}.$$

2. For this system the static gain is given by $G(0) = 1/4$. The time constants are $\tau_1 = 1$ and $\tau_2 = 1/4$ and the damping factor is $\zeta = 5/4$.

Problem 4 (Time response and control) [1 point]

1. The system described by the transfer function $G(s) = \dfrac{4}{18s^2 + 9s + 1}$ possesses the unit step response shown in the following figure. Compute the coordinates of the point M.



2. Design a PID controller for the system in point 1 such that the closed-loop transfer function is $G_{BF}(s) = \dfrac{1}{3s+1}$.

Solution:

1. The unit step response indicates that the system is stable and overdamped ($\zeta > 1$). The static gain is $K = 4$ and the poles are $-\frac{1}{4} \pm \frac{1}{12}$, that is, $-\frac{1}{6}$ and $-\frac{1}{3}$, which means that the time constants are $\tau_1 = 6$ s and $\tau_2 = 3$ s. Then, the inflection point M occurs after

$$t_i = \frac{\tau_1 \tau_2}{\tau_1 - \tau_2} \ln \frac{\tau_1}{\tau_2} = 4.16 \text{ s},$$

and the corresponding time response is

$$y(t_i) = K\left[1 - \frac{\tau_1+\tau_2}{\tau_1}\exp\left(-\frac{\tau_2}{\tau_1-\tau_2}\ln\frac{\tau_1}{\tau_2}\right)\right] = K\left[1 - \frac{\tau_1+\tau_2}{\tau_1}\left(\frac{\tau_1}{\tau_2}\right)^{-\frac{\tau_2}{\tau_1-\tau_2}}\right] = 1.$$

2. The system in point 1 can also be written as

$$G(s) = \frac{K}{(\tau_1 s+1)(\tau_2 s+1)} = \frac{K}{\tau_1\tau_2 s^2 + (\tau_1+\tau_2)s+1},$$

with $K = 4$, $\tau_1 + \tau_2 = 9$ s and $\tau_1\tau_2 = 18$ s.

Therefore, to obtain a closed-loop transfer function $G_{BF}(s) = \dfrac{1}{\tau_{BF}s+1}$ with $\tau_{BF} = 3$, one designs a PID controller with the following parameters:

$$K_R = \frac{\tau_1+\tau_2}{K\tau_{BF}} = 0.75, \qquad \tau_I = \tau_1+\tau_2 = 9 \text{ s}, \qquad \tau_D = \frac{\tau_1\tau_2}{\tau_1+\tau_2} = 2 \text{ s}.$$