

Problem 1 (Modeling) [2 points]

Consider a plug flow reactor of radius r , where the reactions R1 ($2A \rightarrow B$) and R2 ($A+B \rightarrow C$) take place. The concentrations of the chemical species A and B in the feed are denoted as $c_{A,a}$ and $c_{B,a}$, respectively, whereas the temperature in the feed is denoted as T_a . The reaction mixture flows inside the reactor with a velocity v . Its density and heat capacity are constant and equal to ρ and c_p , respectively. The reactor exchanges heat with its wall, which has a constant temperature T_w and an overall heat exchange coefficient (per unit of area) U . The enthalpies of reaction of R1 and R2 (per number of moles of product) are equal to ΔH_1 and ΔH_2 , respectively.

To simplify, let us take into account a small section of length l at the inlet of the reactor and assume that the concentrations of A, B and C in that section are equal to the concentrations at the outlet of that section. Therefore, the concentrations c_A , c_B and c_C and the temperature T represent the states of that section. The reaction rates of R1 and R2 (per unit of volume) are $k_1 c_A^2$ and $k_2 c_A c_B$, respectively.

Write the dynamic model for this section of the reactor.

Solution:

From the mole balance for A

$$\pi r^2 l \dot{c}_A = \pi r^2 v (c_{A,a} - c_A) + \pi r^2 l (-2k_1 c_A^2 - k_2 c_A c_B),$$

one can obtain the dynamic equation for c_A :

$$\dot{c}_A = \frac{v}{l} (c_{A,a} - c_A) - 2k_1 c_A^2 - k_2 c_A c_B$$

Similar mole balances for B and C yield the following dynamic equations for c_B and c_C :

$$\dot{c}_B = \frac{v}{l} (c_{B,a} - c_B) + k_1 c_A^2 - k_2 c_A c_B,$$

$$\dot{c}_C = -\frac{v}{l} c_C + k_2 c_A c_B$$

Finally, from the heat balance

$$\pi r^2 l \rho c_p \dot{T} = \pi r^2 v \rho c_p (T_a - T) + \pi r^2 l (-\Delta H_1 k_1 c_A^2 - \Delta H_2 k_2 c_A c_B) + 2\pi r l U (T_w - T),$$

it is possible to write the dynamic equation for T :

$$\dot{T} = \frac{v}{l} (T_a - T) + \frac{(-\Delta H_1)k_1 c_A^2 + (-\Delta H_2)k_2 c_A c_B}{\rho c_p} + \frac{2U}{r \rho c_p} (T_w - T)$$

Problem 2 (Linearization) [1 point]

Consider the following dynamic equations that describe the concentrations of A and B in a continuous stirred tank reactor:

$$\begin{aligned}\dot{c}_A &= \frac{1}{\theta} (c_{A,a} - c_A) - 2k_1 c_A^2 \\ \dot{c}_B &= -\frac{1}{\theta} c_B + k_1 c_A^2\end{aligned}$$

The following values are constant:

$$\begin{aligned}\theta &= 10 \text{ min} \\ k_1 &= 0.1 \text{ m}^3 \text{ kmol}^{-1} \text{ min}^{-1}\end{aligned}$$

1. Calculate the values of \bar{c}_A and \bar{c}_B at steady state, knowing that $\bar{c}_{A,a} = 10 \text{ kmol m}^{-3}$.
2. Linearize the system around the point calculated in question 1.

Solution:

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

$$\begin{cases} 0 = 0.1 (10 - \bar{c}_A) - 0.2\bar{c}_A^2 \\ 0 = -0.1\bar{c}_B + 0.1\bar{c}_A^2, \end{cases}$$

whose solution is the following:

$$\begin{cases} \bar{c}_A = \frac{0.1 \pm \sqrt{0.1^2 + 4 \times 0.2 \times 1}}{-0.4} = \frac{-1 \pm 9}{4} \\ \bar{c}_B = \bar{c}_A^2 \end{cases} \Rightarrow \begin{cases} \bar{c}_A = 2 \text{ kmol m}^{-3} \\ \bar{c}_B = 2^2 = 4 \text{ kmol m}^{-3} \end{cases}$$

2. In the dynamic model given above, the only (nonlinear) term that needs to be linearized is c_A^2 . It is known that:

$$\left[\frac{\partial}{\partial c_A} (c_A^2) \right]_{c_A=\bar{c}_A} = 2\bar{c}_A$$

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

$$\begin{cases} \delta \dot{c}_A = \frac{1}{\theta} (\delta c_{A,a} - \delta c_A) - 4k_1 \bar{c}_A \delta c_A \\ \delta \dot{c}_B = -\frac{1}{\theta} \delta c_B + 2k_1 \bar{c}_A \delta c_A \end{cases}$$

Problem 3 (Laplace transform) [1 point]

Consider the following dynamic system:

$$\begin{aligned}\ddot{y}_1 + \alpha_1 \dot{y}_1 + \dot{y}_2 &= -u_1 \\ \ddot{y}_2 - \alpha_2 \dot{y}_2 &= \dot{u}_1 - u_2\end{aligned}$$

with all initial conditions zero.

1. Compute the transfer functions: $\frac{Y_1(s)}{U_1(s)}$, $\frac{Y_1(s)}{U_2(s)}$, $\frac{Y_2(s)}{U_1(s)}$, $\frac{Y_2(s)}{U_2(s)}$.
2. Compute the impulse responses for the transfer function $\frac{Y_2(s)}{U_1(s)}$.

Solution:

Applying the Laplace transforms to the two equations:

$$\begin{aligned}s^2 Y_1(s) + \alpha_1 s Y_1(s) + s Y_2(s) &= -U_1(s) \\ s^2 Y_2(s) - \alpha_2 s Y_2(s) &= s U_1(s) - U_2(s)\end{aligned}$$

The last equation gives:

$$\begin{aligned}(s - \alpha_2) s Y_2(s) &= s U_1(s) - U_2(s) \\ Y_2(s) &= \frac{1}{s - \alpha_2} U_1(s) - \frac{1}{s(s - \alpha_2)} U_2(s)\end{aligned}$$

We can then identify $Y_1(s)$ as,

$$\begin{aligned}s(s + \alpha_1) Y_1(s) &= -U_1(s) - s Y_2(s) \\ Y_1(s) &= \frac{-U_1(s)}{s(s + \alpha_1)} - \frac{Y_2(s)}{(s + \alpha_1)} \\ Y_1(s) &= \frac{\alpha_2 - 2s}{s(s + \alpha_1)(s - \alpha_2)} U_1(s) + \frac{1}{s(s + \alpha_1)(s - \alpha_2)} U_2(s)\end{aligned}$$

The transfer functions can then be written as:

$$\frac{Y_1(s)}{U_1(s)} = \frac{\alpha_2 - 2s}{s(s + \alpha_1)(s - \alpha_2)}$$

$$\frac{Y_1(s)}{U_2(s)} = \frac{1}{s(s + \alpha_1)(s - \alpha_2)}$$

$$\frac{Y_2(s)}{U_1(s)} = \frac{1}{s - \alpha_2}$$

$$\frac{Y_2(s)}{U_2(s)} = \frac{-1}{s(s - \alpha_2)}$$

For the impulse response, we have $U_1(s) = 1$. Using the method of residuals and taking inverse Laplace transform gives:

$$y_2(t) = e^{\alpha_2 t}$$

Note: The system is stable only when $\alpha_2 < 0$.

Problem 4 (Control) [1 point]

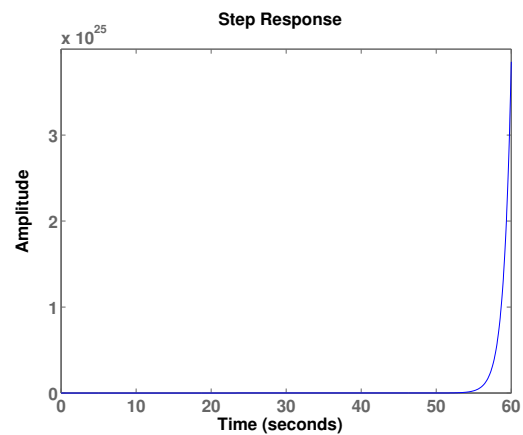
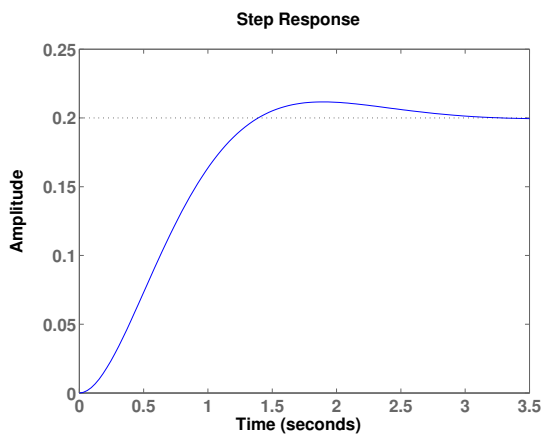
- Determine whether the systems described by the following transfer functions are stable:

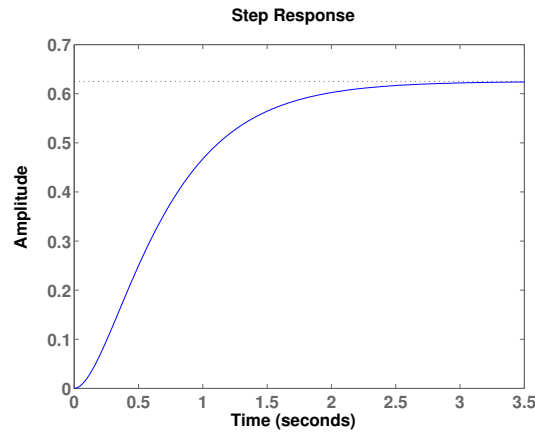
(a) $G(s) = \frac{5}{(s+2)(s+4)}$

(b) $G(s) = \frac{1}{s^2+s-2}$

(c) $G(s) = \frac{1}{s^2+3s+5}$

- Match the transfer functions given above with the step responses shown in the following figures:





3. Design a PI controller and a PID controller for the following system:

$$G(s) = \frac{e^{-2s}}{3s+1}$$

Solution:

1) In order to check the stability of the system, we compute the poles of the system. If the poles are in the negative side of the complex plane, then the system is stable.

- a) The poles are -2 and -4. The system is stable.
- b) The poles are 1 and -2. The system is unstable.
- c) The system has complex poles with negative real parts. Hence the system is stable.

2) We can clearly match the step response based on the computed poles.

- a) We see that the step response is stable and has oscillations. This corresponds to a system with complex poles, namely, $G(s) = \frac{1}{s^2+3s+5}$
- b) The step response tends to infinity. Hence the system is unstable. $G(s) = \frac{1}{s^2+s-2}$
- c) The step response is devoid of oscillations and is stable. $G(s) = \frac{5}{(s+2)(s+4)}$

3) Design of PI and PID controller:

We can use the ZN - method for designing the controllers.

PI Controller:

$$K_R = 0.9 \frac{\tau}{\theta K} = 1.35$$

$$\tau_I = 3.33\theta = 6.66$$

PID Controller:

$$K_R = 1.2 \frac{\tau}{\theta K} = 1.80$$

$$\tau_I = 2\theta = 4$$

$$\tau_D = 0.5\theta = 1$$