Problem 1 (Modeling) [2 points]

Consider a vessel with a binary mixture of species A and B in the liquid and vapor phases. The number of moles in the liquid phase is denoted as \( n \), and the molar fractions of A in the liquid phase and in the vapor phase are \( x_A \) and \( y_A \). The vapor phase is in equilibrium with the liquid phase, and this equilibrium is given by the equation \( y_A = \frac{\alpha x_A}{1 + (\alpha - 1)x_A} \). The reaction \( A \rightarrow B \) takes place in the liquid phase, and the reaction rate (per unit of volume) is \( kc_A \) with \( c_A = \frac{n_A}{V_l} \), where \( n_A \) is the number of moles of A in the liquid phase and \( V_l \) is the volume of the liquid phase.

The inlet of the liquid phase is composed of a mixture of A and B with a molar fraction \( z_A \) of A, and its molar flowrate is denoted as \( F \). The outlet molar flowrate of the liquid phase, denoted as \( L \), is equal to \( C\sqrt{n} \). Since there is no accumulation in the vapor phase, the outlet molar flowrate of the vapor phase is equal to the molar flowrate that is vaporized from the liquid phase, denoted as \( V \). The outlet of the vapor phase is cooled down in a condenser where there is no accumulation, which means that the composition of the outlet of the condenser is the same as the composition of the vapor phase in the vessel. A part of the outlet of the condenser, whose molar flowrate is equal to \( D \), leaves the process, whereas the other part of the outlet of the condenser is recycled to the liquid phase of the vessel.

Write the dynamic model for this vessel using \( n \) and \( x_A \) as state variables.
Solution:

A molar balance for the liquid phase of the vessel gives the following differential equation, which describes the evolution of the state variable $n$:

$$
\dot{n} = F + (V - D) - V - L = F - D - C\sqrt{n}.
$$

A molar balance for A in the liquid phase of the vessel gives

$$
\dot{n}_A = -V_l k \frac{n_A}{V_l} + F z_A + (V - D) y_A - V y_A - L x_A =
$$

$$
= -k n x_A + F z_A - D \frac{\alpha x_A}{1 + (\alpha - 1) x_A} - C \sqrt{n} x_A.
$$

Since

$$
\dot{n}_A = \dot{x}_A n + \dot{n} x_A,
$$

the differential equation that describes the evolution of the state variable $x_A$ is

$$
\dot{x}_A = \frac{\dot{n}_A - \dot{n} x_A}{n} = -k x_A + \frac{F}{n} (z_A - x_A) - \frac{D}{n} \left( \frac{\alpha x_A}{1 + (\alpha - 1) x_A} - x_A \right).
$$

Therefore, the dynamic model of the vessel is represented by the differential equations

$$
\dot{n} = F - D - C\sqrt{n},
$$

$$
\dot{x}_A = -k x_A + \frac{F}{n} (z_A - x_A) - \frac{D}{n} \left( \frac{\alpha x_A}{1 + (\alpha - 1) x_A} - x_A \right).
$$
Problem 2 (Linearization) [1 point]

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

\[
\dot{c}_A = \frac{1}{\theta} (c_{A,e} - c_A) - k_1 c_A \sqrt{c_B}, \\
\dot{c}_B = -\frac{1}{\theta} c_B + k_1 c_A \sqrt{c_B},
\]

with the numerical values \(\theta = 10\) min, \(k_1 = 0.2\) m\(^{1.5}\) kmol\(^{-0.5}\) min\(^{-1}\).

1. Calculate the values \(\bar{c}_A\) and \(\bar{c}_B\) at steady state, knowing that \(c_{A,e} = 5\) kmol m\(^{-3}\).

2. Linearize the system around the point calculated in point 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

\[
\begin{align*}
0 &= 0.1 \left(5 - \bar{c}_A\right) - 0.2 \bar{c}_A \sqrt{\bar{c}_B} \\
0 &= -0.1 \bar{c}_B + 0.2 \bar{c}_A \sqrt{\bar{c}_B}
\end{align*}
\]

\[
\implies \begin{cases} 
0 = 0.1 \left(5 - \bar{c}_A\right) - 0.2 \bar{c}_A \sqrt{\bar{c}_B} = 0.5 - 0.1 \bar{c}_A - 0.4 \bar{c}_A^2 \\
0 = -0.1 \bar{c}_B + 0.2 \bar{c}_A \sqrt{\bar{c}_B} = 2 \bar{c}_A
\end{cases}
\]

whose solution is the following:

\[
\begin{cases} 
\bar{c}_A = \frac{0.1 \pm \sqrt{0.1^2 + 4 \times 0.4 \times 0.5}}{-0.8} = \frac{-1 \pm 9}{8} \\
\bar{c}_B = 4 \bar{c}_A^2
\end{cases}
\]

\[
\implies \begin{cases} 
\bar{c}_A = 1\ \text{kmol}\ m^{-3} \\
\bar{c}_B = 4\ \text{kmol}\ m^{-3}
\end{cases}
\]

2. In the dynamic model given above, the only (nonlinear) term that needs to be linearized is \(c_A \sqrt{c_B}\). It is known that

\[
\left[ \frac{\partial}{\partial c_A} (c_A \sqrt{c_B}) \right]_{c_A = \bar{c}_A, c_B = \bar{c}_B} = \sqrt{\bar{c}_B},
\]

\[
\left[ \frac{\partial}{\partial c_B} (c_A \sqrt{c_B}) \right]_{c_A = \bar{c}_A, c_B = \bar{c}_B} = \frac{\bar{c}_A}{2 \sqrt{\bar{c}_B}}.
\]

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

\[
\begin{align*}
\delta \dot{c}_A &= \frac{1}{\theta} \left(\delta c_{A,e} - \delta c_A\right) - k_1 \sqrt{\bar{c}_B} \delta c_A - k_1 \frac{\bar{c}_A}{2 \sqrt{\bar{c}_B}} \delta c_B \\
\delta \dot{c}_B &= -\frac{1}{\theta} \delta c_B + k_1 \sqrt{\bar{c}_B} \delta c_A + k_1 \frac{\bar{c}_A}{2 \sqrt{\bar{c}_B}} \delta c_B
\end{align*}
\]
Problem 3 (Laplace transform) [1 point]

A process is described by the differential equation

\[3\dot{y}(t) + y(t) = u(t - 0.1), \quad y(0) = 0,\]

where \(u\) is the input and \(y\) is the output.

1. Calculate the transfer function using Laplace transform. What are the static gain, the time constant, and the pure delay of the process?

2. Calculate the impulse response.

Solution:

1. Performing Laplace transform gives

\[3sY(s) + Y(s) = e^{-0.1s}U(s),\]
\[Y(s) = \frac{e^{-0.1s}}{3s + 1}U(s).\]

For this process the static gain is given by \(G(0) = 1\). The time constant is \(\tau = 3\) and the pure delay is 0.1.

2. For an impulse response, \(U(s) = 1\), hence

\[Y(s) = \frac{e^{-0.1s}}{3s + 1}.\]

Taking inverse Laplace transformation gives

\[y(t) = \begin{cases} 0, & t < 0.1 \\ \frac{1}{3}e^{-(t-0.1)/3}, & t \geq 0.1 \end{cases} \]
Problem 4 (Time responses and control) [1 point]

1. Consider the systems described by the following transfer functions:

(i) \( G(s) = \frac{1.25(s+0.8)e^{-3s}}{(6s+1)^2} \)

(ii) \( G(s) = \frac{-4s+1}{(6s+1)^2} \)

(iii) \( G(s) = \frac{1.25}{(6s+1)^2} \)

(iv) \( G(s) = \frac{4.5}{s^2+9} \)

(v) \( G(s) = \frac{1.25}{9s^2+3s+1} \)

Match the transfer functions given above with the step responses shown in the following figure:
2. Consider the feedback system used to reject the disturbance $d$ shown in the following figure:

![Feedback System Diagram]

Given that $G(0) = \frac{7}{3}$, $Y_c(s) = 0$ and the disturbance $d$ is a unit step, calculate the steady-state error $e(\infty)$ as a function of $K$.

**Solution:**

1. The step responses corresponding to different transfer functions are:
   (i) $b$
   (ii) $e$
   (iii) $c$
   (iv) $a$
   (v) $d$

2. The transfer function of the system is,

   $$E(s) = -G(s)(D(s) + KE(s)),$$

   $$E(s) = \frac{-G(s)}{1 + KG(s)} D(s).$$

Now $D(s) = \frac{1}{s}$ gives,

$$e(\infty) = \lim_{s \to 0} sE(s) = \frac{-G(0)}{1 + KG(0)} = \frac{-7/3}{1 + 7K/3},$$

The steady-state error decreases with larger $K$. 