Consider a constant volume isothermal CSTR in which the following series-parallel reaction known as the van de Vusse reaction scheme takes place:

\[ A \xrightleftharpoons{k_1} B \xrightleftharpoons{k_2} C \]
\[ 2A \xrightarrow{k_3} D \]

The intermediate component \( B \) in the series reaction is the desired product. The molar rate of formation (per unit volume) of each component is

\[
\begin{align*}
r_A &= -k_1 C_A - k_3 C_A^2 \\
r_B &= k_1 C_A - k_2 C_B \\
r_C &= k_2 C_B \\
r_D &= \frac{1}{2} k_3 C_A^2
\end{align*}
\]

The dynamic model equations are:

\[
\begin{align*}
\frac{dC_A}{dt} &= \frac{F}{V} (C_{Af} - C_A) - k_1 C_A - k_3 C_A^2 \\
\frac{dC_B}{dt} &= -\frac{F}{V} C_B + k_1 C_A - k_2 C_B
\end{align*}
\]

where \( F/V \) is the dilution rate, \( C_X \) is the concentration of component \( X \), and \( k_i \) is the rate constant for the \( i^{th} \) reaction. Notice that neither of the equations depend on the concentration of component \( C \) or \( D \). Since we are only concerned about the concentration of \( B \), the balances for the other two components are not needed.

1. Consider the following parameter values: \( k_1 = 5/6 \text{ min}^{-1}, k_2 = 5/3 \text{ min}^{-1}, k_3 = 1/6 \text{ mol L}^{-1} \text{ min} \), and \( C_{Af} = 10 \text{ mol L}^{-1} \). Find the optimum achievable steady-state concentration of \( B \) analytically for the case where the dilution rate \( (F/V) \) is the manipulated input.

2. Verify the optimum graphically by constructing a steady-state input-output curve relating \( F/V \) and \( C_B \). Comment on the nonlinear relationship between the input and the output.

3. Build an open-loop Simulink model with the dilution rate \( (F/V) \) as the input and concentration of \( B \) \( (C_B) \) as the output.
4. The maximum achievable concentration of $B$ corresponds to a singularity, and the system is uncontrollable at this point. Instead consider both of the steady states corresponding to $C_B = 1.117 \text{ mol/L}$ ($F/V = 0.5714 \text{ min}^{-1}$ and $F/V = 2.8744 \text{ min}^{-1}$). Use your open-loop Simulink model to find the linear state-space model for both steady-state operating points.

5. Compute the eigenvalues of each state-space model and determine the stability of each steady state.

6. Use Matlab to find the transfer function $G(s) = C_B(s)/D(s)$ corresponding to each state-space model ($D \equiv F/V$).

7. Find the zeros and poles of each transfer function model and determine the stability of each steady state.

8. Use the direct substitution method and the transfer function models to analytically determine the ultimate controller gain ($K_{cu}$) for each steady state.

9. Build a closed-loop Simulink model for control of the concentration of $B$ ($C_B$) by manipulation of the dilution rate ($F/V$). Use the closed-loop simulation to determine the ultimate controller gain ($K_{cu}$) near the steady state corresponding to $F/V = 0.5714 \text{ min}^{-1}$. Make a small step change away from the steady state to slightly perturb the system.

10. Use the ultimate gain found by simulation and the Ziegler-Nichols tuning method to find PI controller parameters.

11. Evaluate the PI controller parameters. Consider step changes in the concentration setpoint $C_B (+/− 0.1 \text{ mol/L})$ and the feed concentration $C_{Af} (+/− 1.0 \text{ mol/L})$ for a system initially at the steady-state where $F/V = 0.5714 \text{ min}^{-1}$.

12. Use Skogestad’s method to find a first-order-plus-time-delay (FOPDT) model that approximates the higher order transfer function corresponding to the steady state at $F/V = 0.5714 \text{ min}^{-1}$.

13. Use your FOPDT model and the Tyreus-Luyben tuning relations to determine an additional set of PI controller parameters.

14. Consider step-changes in the concentration setpoint $C_B$ to compare the performance of the PI parameters determined from the Tyreus-Luyben tuning relations with the ones previously determined by the Ziegler-Nichols tuning method.