

## Homework 01 – Simulation of Dynamic Systems

Otacilio “Minho” Neto (otacilio.bneto@pm.me)

## Problem Setup

A CSTR of constant volume  $V$  implements the exothermic reaction  $A \xrightarrow{\kappa(T)} B$  in liquid phase (Figure 1). Using mass balance equations, the dynamics of the concentrations  $c_A$  and the temperature  $T$  are modelled as

$$V \frac{d}{dt} c_A = q(c_{Ai} - c_A) - V\kappa(T)c_A \quad (1a)$$

$$V\rho C \frac{d}{dt} T = \rho C q(T_i - T) + V(-\Delta H_R)\kappa(T)c_A + UA(T_c - T) \quad (1b)$$

with kinetic rate  $\kappa(T) = \kappa_0 \exp(-\frac{E}{RT})$ . The model parameters ( $V, c_{Ai}, T_i, k_0, \frac{E}{R}, -\Delta H_R, C, \rho, UA$ ) are in Table 1.

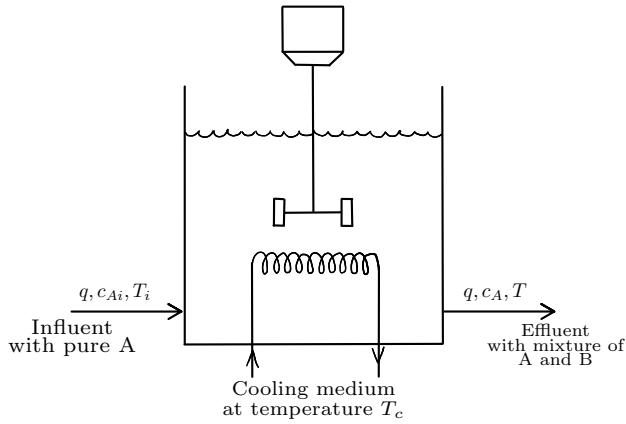


Figure 1. Exothermic CSTR: Process layout.

| Variable      | Description [Units]              | Value  |
|---------------|----------------------------------|--------|
| $E$           | Activation energy [J/gmol]       | 72750  |
| $R$           | Gas constant [J/gmol/K]          | 8.314  |
| $\kappa_0$    | Arrhenius rate constant [1/min]  | 7.2e10 |
| $V$           | Volume [L]                       | 100    |
| $\rho$        | Density [g/L]                    | 1000   |
| $C$           | Heat capacity [J/g/K]            | 0.239  |
| $-\Delta H_R$ | Enthalpy of reaction [J/mol]     | 5.0e4  |
| $UA$          | Heat transfer [J/min/K]          | 5.0e4  |
| $c_{Ai}$      | Inlet feed concentration [mol/L] | 1      |
| $T_i$         | Inlet feed temperature [K]       | 350    |

Table 1. Exothermic CSTR: Model constant parameters.

Using control notation, the state signal is  $x = (x_1, x_2) = (c_A, T)$  and the control signal is  $u = (u_1, u_2) = (q, T_c)$ . In this homework, you will simulate the dynamics of this system for different input signals. Rewrite the model in Eq. (1a)-(1b) using the control notation to have it in the form  $\frac{d}{dt}x(t) = f(x(t), u(t))$ , then solve the following tasks:

**Task 1. (10 points)** Using the Runge-Kutta 4th-Order (RK4) method, simulate the state response  $x(t)$ , for  $t \in [0, T]$ , of the exothermic CSTR given the initial state  $x(0) = (0.5, 350)$  and control signals

$$u_1(t) = \begin{cases} 100 & \text{if } t \leq T/4 \\ 112 & \text{if } t > T/4 \end{cases} \quad \text{and} \quad u_2(t) = \begin{cases} 305 & \text{if } t \leq 3T/4 \\ 300 & \text{if } t > 3T/4 \end{cases}. \quad (2)$$

Use a discretization period  $\Delta t = 0.01$  (or smaller) and a simulation horizon  $T = 24\text{min}$  (or larger). **Comment on the results:** What interesting dynamical behaviors do you observe? How is the generation of the chemical B (i.e., the consumption of A) affected by the changes in the inputs?

**Task 2. (10 points)** Linearize the model  $\frac{d}{dt}x(t) = f(x(t), u(t))$  around the steady-state pair  $(x_{\text{ref}}, u_{\text{ref}})$  given by

$$x_{\text{ref}} = \begin{bmatrix} 0.094341 \\ 386.75607 \end{bmatrix} \quad \text{and} \quad u_{\text{ref}} = \begin{bmatrix} 112 \\ 305 \end{bmatrix} \quad (3)$$

then simulate the linearized system  $\frac{d}{dt}x^\delta = Ax^\delta + Bu^\delta$  using the same setup from **Task 1**. **Comment on the results:** Are there periods in which the two models produce similar results? Why? What does the linearized matrix  $A$  (i.e., its eigenvalues) tells us about the stability of the operating point  $(x_{\text{ref}}, u_{\text{ref}})$ ?

*Hint: You can use if-else statements or the sign( $\cdot$ ) function to implement the input signal  $u(\cdot)$ . When simulating the linearized system, remember to shift the initial state,  $x^\delta(0) = x(0) - x_{\text{ref}}$ , and the inputs  $u^\delta(t) = u(t) - u_{\text{ref}}$ . When plotting, use  $x(t) = x_{\text{ref}} + x^\delta(t)$  and  $u(t) = u_{\text{ref}} + u^\delta(t)$  to have them back to the original variables.*