CHE 4600 - Process Dynamics and Simulation

Control Project: Control of a Chemical Reactor

Assigned: Thursday, November 12

Due: Sunday, December 6 by 11:59 PM

Consider a jacketed continuous stirred tank reactor (CSTR) shown below:

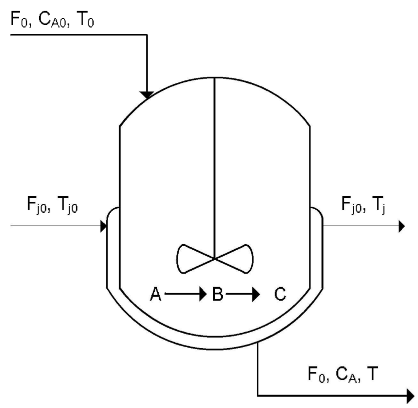

Figure 1: A jacketed continuous stirred tank reactor.

The following group of reactions takes place in the reactor:

$$A \longrightarrow B \longrightarrow C$$

where A to B is a highly exothermic reaction and B to C is a reaction that generates a negligible amount of heat.

The reactor is fed by pure species A at temperature T_0, concentration C_{A0} and flow rate F_0. The effluent stream leaves the reactor at concentrations C_A, C_B, C_C, and temperature T. The jacket is fed by water at temperature T_{j0} and flow rate F_{j0}. The effluent stream leaves the jacket at temperature T_j.

Process model

The material and energy balances that describe the dynamic behavior of the process have the following form:

$$\begin{aligned}
\frac{dC_A}{dt} &= \tfrac{F_0}{V}(C_{A0} - C_A) - k_1 e^{-E_1/(RT)} C_A \\
\frac{dC_B}{dt} &= \tfrac{-F_0}{V} C_B + k_1 e^{-E_1/(RT)} C_A - k_2 e^{-E_2/(RT)} C_B \\
\frac{dT}{dt} &= \tfrac{UA}{\rho C_p V}(T_j - T) + \tfrac{F_0}{V}(T_0 - T) - k_1 e^{-E_1/(RT)} C_A \tfrac{\Delta H_1}{\rho C_p} - k_2 e^{-E_2/(RT)} C_B \tfrac{\Delta H_2}{\rho C_p} \\
\frac{dT_j}{dt} &= \tfrac{F_{j0}}{V_j}(T_{j0} - T_j) + \tfrac{UA}{\rho_j C_{pj} V_j}(T - T_j)
\end{aligned} \qquad (1)$$

where:

C_A: concentration of species A in the reactor

C_B: concentration of species B in the reactor

T: temperature of the reactor
T_j: temperature of the jacket
T_0: temperature of reactor inlet stream
T_{j0}: temperature of jacket inlet stream
t: dimensionless time

Model parameters are presented in Table 1.

Table 1: Parameters for the CSTR.

Parameter	**Description**	**Value**	**Units**
UA	Overall heat transfer coefficient*Heat exchange area	1200	$\frac{kJ}{h \cdot K}$
ρ	Density of fluid in CSTR	1200	$\frac{kg}{m^3}$
C_p	Heat capacity of fluid in CSTR	0.42	$\frac{kJ}{kg \cdot K}$
ρ_j	Density of fluid in jacket	1000	$\frac{kg}{m^3}$
C_{pj}	Heat capacity of fluid in jacket	4.18	$\frac{kJ}{kg \cdot K}$
k_1	Pre-exponential factor, Reaction 1	6×10^5	$\frac{m^3 \cdot h}{kmol}$
k_2	Pre-exponential factor, Reaction 2	2×10^6	$\frac{m^3 \cdot h}{kmol}$
E_1	Activation energy, Reaction 1	5×10^4	$\frac{kJ}{kmol}$
E_2	Activation energy, Reaction 2	5.5×10^4	$\frac{kJ}{kmol}$
C_{A0}	Inlet stream concentration of A	7	$\frac{kmol}{m^3}$
T_0	Inlet stream temperature	300	K
F	Flow rate through CSTR	4	$\frac{m^3}{h}$
F_j	Flow rate through jacket	1	$\frac{m^3}{h}$
T_{j0}	Jacket inlet stream temperature	240	K
ΔH_1	Heat of reaction, Reaction 1	-2×10^4	$\frac{kJ}{kmol}$
ΔH_2	Heat of reaction, Reaction 2	-3×10^4	$\frac{kJ}{kmol}$
V	CSTR volume	6	m^3
V_j	Jacket volume	5	m^3
R	Gas constant	8.314	$\frac{kJ}{kmol \cdot K}$

Specific Questions

1. (10 pts.) Examples of some steady-states are listed in Table 2. Determine the stability of each of these steady-states via linearization around the steady-states and describe how you determined it. Include any code used to determine this in an appendix.

Table 2: Two CSTR Steady-States. Concentrations are in kmol/m^3. Temperatures are in K.

C_A	C_B	C_C	T	T_j
0.0226301208683143	0.0150450773785251	6.96232480175316	753.722140349192	354.584864018407
6.99677782598635	0.00322159294563358	5.81073225911324e-07	281.113901760693	249.17038700984

2. (15 pts.) Assume that operation around the unstable steady-state operating condition is preferable. Using temperature of the reactor as the controlled and measured output ($\bar{y}$ in deviation variable form),

temperature of the jacket inlet stream as the manipulated input ($\bar{u}$ in deviation variable form), and temperature of the reactor inlet stream as the disturbance ($\bar{d}$ in deviation variable form), compute the transfer function of the linearized system in deviation variable form. Show the linearized system in your report and key steps in computing the transfer function, with a description of how to go from one key step to the next. It should be clear that you know how to derive the transfer function completely from what you choose to present.

3. (15 pts.) Describe the steps in how to get the closed-loop transfer function from that in the prior part, and write the form of the closed-loop transfer function when a P controller is used. It should be clear that you know how to derive the transfer function completely from what you choose to present. For a P controller, what values of K_c are needed to ensure that the closed-loop system is stable?

4. (20 pts.) Design a proportional-integral (PI) controller to stabilize the closed-loop system resulting from the linearized system and the controller. Explain how you chose the PI controller tuning parameters.

5. (20 pts.) Apply the PI controller to the linearized system and the nonlinear system of Eq. 1, for set-point changes in the reactor temperature, $\bar{y}$, of magnitude 0.005 and 1 (show the plots of the manipulated input and the controlled output for all the simulation runs). Explain why similarities and differences between the plots exist.

6. (20 pts.) Study the disturbance rejection capabilities of the controller, for step changes in the temperature of the reactor inlet stream, $\bar{d}$, of magnitude 0.001 and 0.05. Consider both the linearized system and the nonlinear system (show the plots of the manipulated input and the controlled output for all the simulation runs). Explain why similarities and differences between the plots exist.

Statements must be accurate and precise.

There is no maximum/minimum required length. Reports must be comprehensive and accurately and thoroughly address all points above, or points may be removed. Please use single spacing. Type this report.

You are expected to work independently on the project. In order to do the simulation part of the project, you can write your own code using MATLAB. You can perform the numerical integration yourself or use a built-in MATLAB solver like ode45 if desired.

Requirements for Formatting and Report-Writing

In your future job, whether you go to graduate school and continue in academia, or whether you go to industry, the task that you are likely to spend the greatest amount of time on is communicating. You will communicate with your colleagues in person every day, but you will also do a significant amount of written communication, via email and via written reports. As an engineer, *what you say matters.* You will be trusted with making decisions and backing them up. You need to make sure that you are precise and thorough in what you say. Any email or report that you write may be forwarded to customers or to other colleagues (especially higher-level management), whether you know that it has been or not. You will have projects that go on and on for years, where someone will ask you one day why you did something a few months or even years ago, and the only way you will remember that is if you documented the decision in a way that you can pick up again the report or email you wrote at the time and feel very clear, without any doubt, of how you arrived at your conclusion. Therefore, it is crucial that you learn to express what you have done clearly.

Your company or group will likely have a format that they use to send out major reports, and you will use that. If you are not given a structure, you have some freedom, but it is good to present in a logical fashion. In this paper, I have provided a structure. However, in addition to the structure, the following requirements must be met (up to 5 points will be deducted for violations of these requirements or poor writing):