Process Dynamics Portfolio:
A First Look at Process Dynamics with MATLAB Simulations

Course: CHE 322

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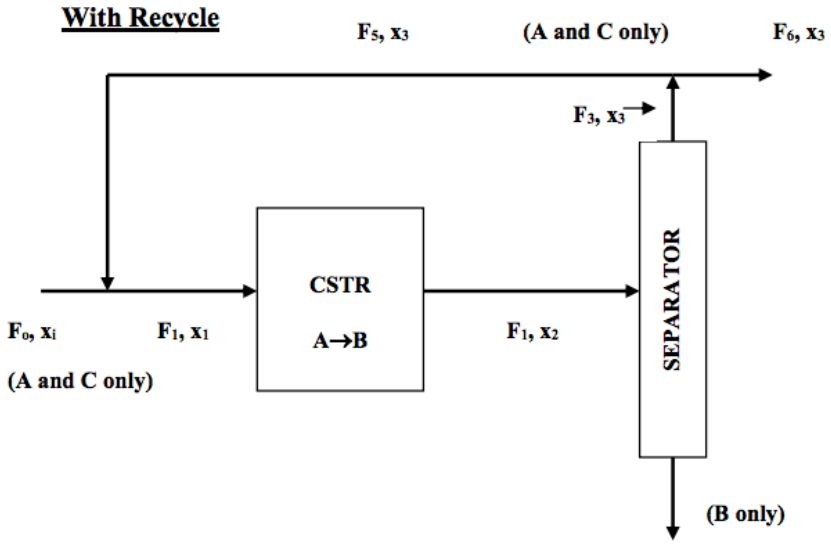
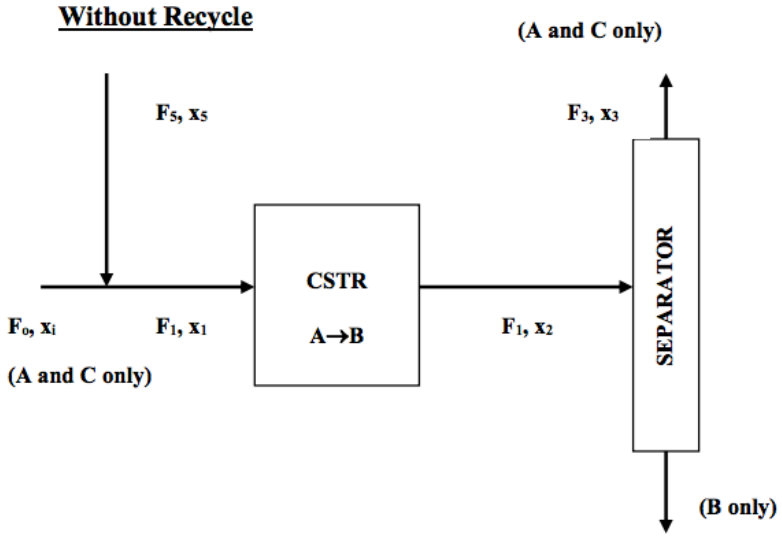
Portfolio 1

Note: All compositions (x_i, x_1, x_2, x_3) are referring to compositions of component A.

Block Flow Diagrams (From Portfolio Problem #1 Document)





ii) Model equations, assumptions, and a complete set of steady-state data for recycle and without recycle cases.

Mixing Point

$$F_1 = F_o + F_5$$
$$F_1 x_{1,A} = F_o x_{i,A} + F_5 x_{3,A} \qquad (1)$$

CSTR

$$\frac{d(Mx_{2,A})}{dt} = F_1 x_{1,A} - F_1 x_{2,A} - k_o x_{2,A} M$$

or

$$\frac{dx_{2,A}}{dt} = \frac{1}{\tau}(x_{1,A} - x_{2,A}) - k_o x_{2,A} \qquad (2)$$

$$\tau = \frac{M}{F_1}$$

Separator

$$F_1 x_{2,A} = F_3 x_{3,A} \qquad (3)$$

Assumptions:

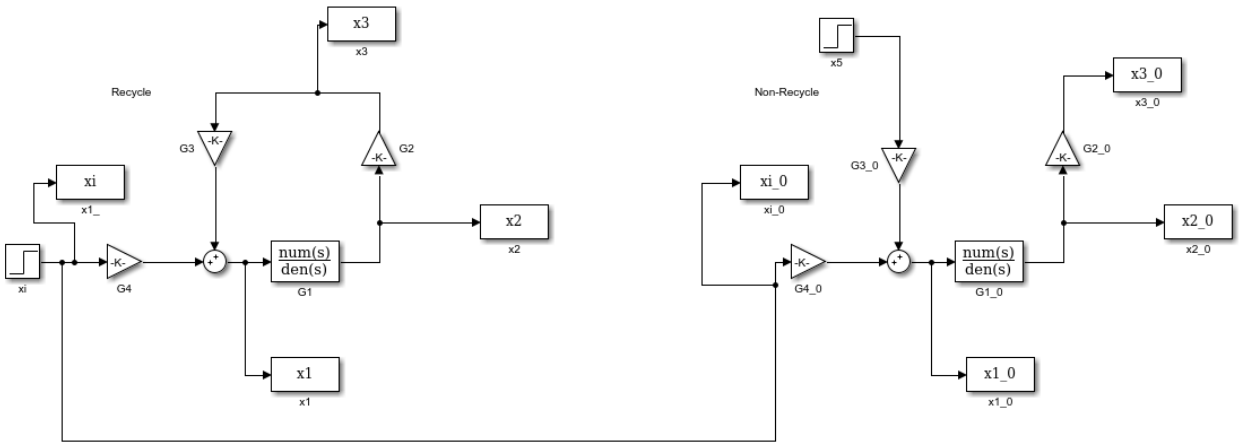
(1) Constant molar holdup (M) in CSTR – M is taken out of the derivative in the CSTR balance
(2) All molar flowrates remain constant – Flowrates are not modelled with differential equations
(3) Perfect separation unit with infinitely fast dynamics – No delay in separator equation: inlet = outlet
(4) No transportation delay between separator and feed-recycle mixing point – x3 is used interchangeably with x5
(5) Isothermal process – constant rate constant, which is a function of temperature

Steady State Data:

$x_i = 0.95$
$x_1 = 2/3$
$x_2 = 1/3$
$x_3 = 0.5$

See Appendix A for calculations and the MATLAB code

iii) Parts c) and d) including both block diagrams and all individual transfer functions.



$$G1 = \frac{1/\tau}{s+1/\tau+k_oM} = \frac{(1/\tau)\left(\frac{1}{(1/\tau+k_oM)}\right)}{s\left(\frac{1}{(1/\tau+k_oM)}\right)+1}$$

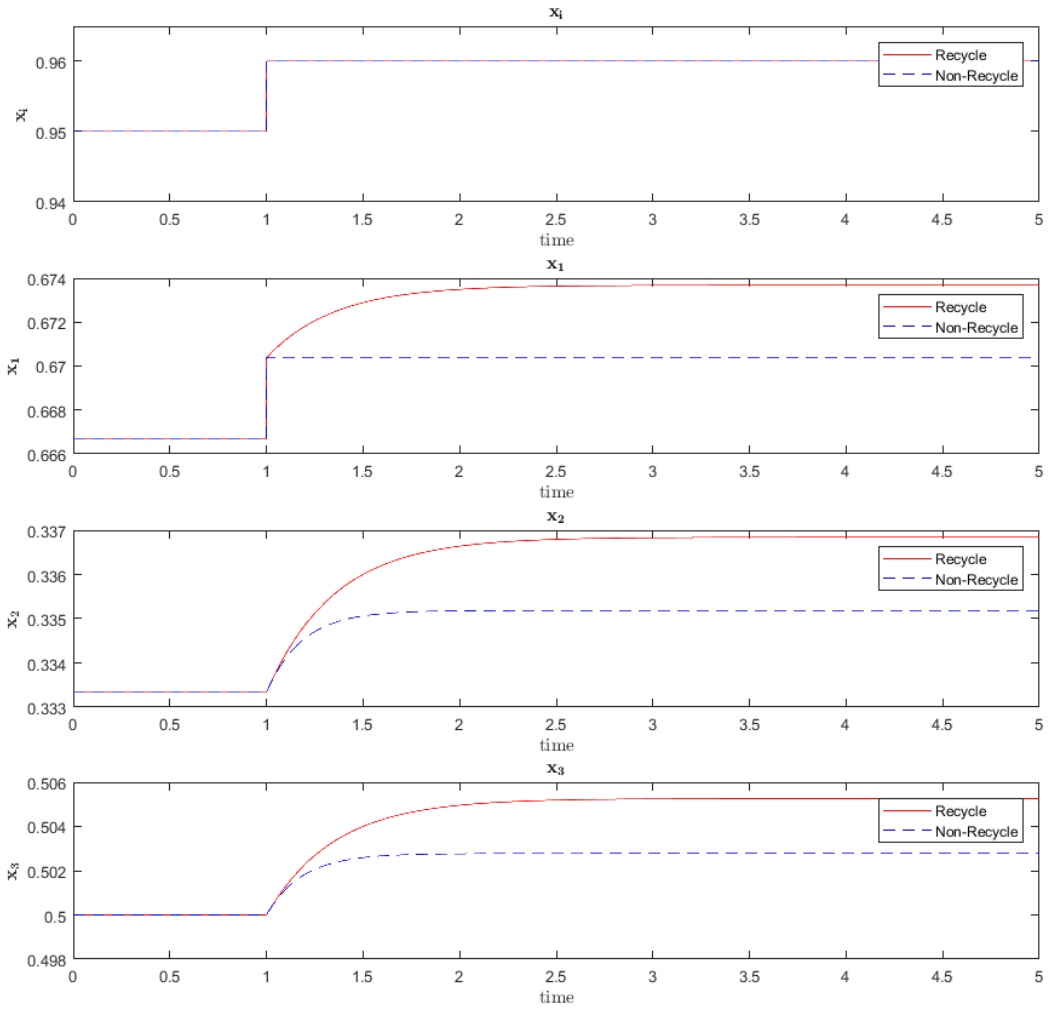
G2 = F_1/F_3

G3 = F_5/F_1

G4 = F_o/F_1

iv) Simulation results from part f) with subplot(41#) showing original variables in the order indicated. Figure must use different line types and a legend to distinguish between recycle and without recycle cases and must be properly labeled.

Step change in x_i from 0.95 to 0.96:



v) Based on the results from part f), provide a chemical engineering explanation for the differences in the behaviour of the two cases.

In the non-recycle CSTR, the additional amount of A in the feed goes through the reactor just once. The amount of A in the outlet (x_2) has increased, because not all of the additional A reacted to form B. For each additional amount of feed to any reactor, only a fraction will be converted. For the recycle CSTR, the recycle string brings component A back to the start of the system, raising x_1. Entering the CSTR with a higher x_1, as explained, results in a higher amount of A exiting the CSTR, raising x_2 and x_3. This is why x_2 and x_3 are higher for the recycle CSTR – A is not "lost" in stream 3, it is kept in the cycle, increasing overall reactor performance.

Just looking at x_1, the response is immediate for the non-recycle system. In this system, there is no recycle stream affecting x_1. In the recycle CSTR, the recycle stream changes the CSTR inlet, so the x_1 has to reach a new steady state based on the recycle achieving steady state. By looping through the system, it takes longer to achieve steady state, which can be seen in x_1, x_2, and x_3.

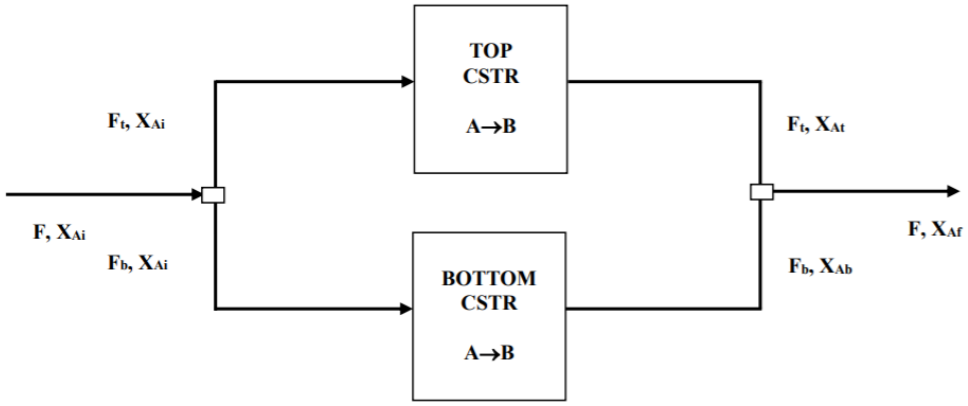
vi) Based on the results from part f), provide a process dynamics and control explanation for the differences in the behaviour of the two cases.

The non-recycle CSTR is mainly a system in series. Any changes are felt downstream but not upstream of the change. Therefore, changing x_i will of course affect x_1 and everything further downstream. However, since there is nothing else being changed upstream of x_1, the change in x_1 is immediate. In the recycle CSTR, there are multiple transfer functions, G1, G2, G3 that are changing x_1, and also feeding back into x_1. This is a feedback system. A feedback system is slow when the feedback loop is very large, and it is always slower than a series setup. This is why whenever one is controlling a system, the measured system input should be as close as possible to the controlled variable. This is why the dynamics are slower for the recycle CSTR.

The reason why the steady state values are higher for the recycle CSTR is because component A is going through the gain blocks/transfer functions multiple times. The recycle stream brings the additional A after the separator back through G3 and back into G1, increasing the final amounts of x_1, x_2, and x_3.

Portfolio 2

i)



ii)

TOP CSTR

$$\frac{dX_{At}}{dt} = \frac{F_t}{M_t}(X_{Ai} - X_{At}) - k_t X_{At}$$

BOTTOM CSTR

$$\frac{dX_{Ab}}{dt} = \frac{F_b}{M_b}(X_{Ai} - X_{Ab}) - k_b X_{Ab}$$

MIXER

$$F_t X_{At} + F_b X_{Ab} = F\ X_{Af}$$

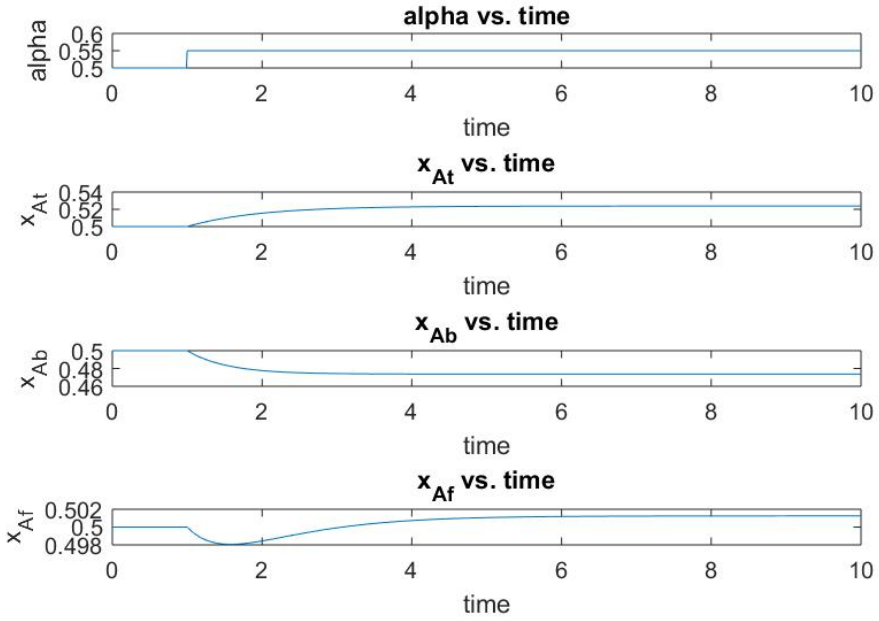
Assumptions
(1) Constant molar holdups in CSTR's

(2) Isothermal process

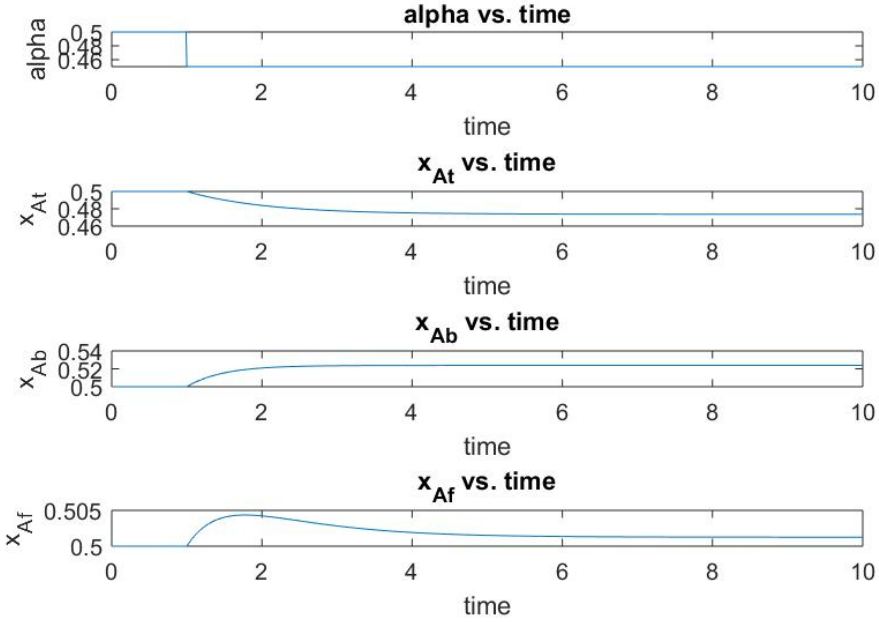
Steady State Values:
F=1 (moles/time)
$F_t=\alpha=0.5$ (moles/time)
$F_b=1-\alpha=0.5$ (moles/time)
$x_{Ai}=1.0$ $M_t=1$ mole
$M_b=0.5$ mole
$k_t=0.5$ (time^{-1})
$k_b=1.0$ (time^{-1}) $x_{At}=0.5$
$x_{Ab}=0.5$
$x_{Af}=0.\ 5$

iii)

Split fraction from 0.5 to 0.55:



Split fraction from 0.5 to 0.45:



iv) Increasing the split fraction causes the final mole fraction to initially decrease and then increase back until a new steady state is reached. A greater split fraction results in a higher flowrate going into the top CSTR and lower flowrate to the bottom CSTR, which causes the top CSTR to have a lower residence time and therefore lower conversion (x_A increases). Conversely, the bottom CSTR will have a greater residence time and higher conversion (x_A decreases). The faster rate of change of x_A in the bottom CSTR (decreasing x_A) and slower rate of change in the top CSTR (increasing x_A) accounts for the initial dip of the final mole fraction. As the top CSTR catches up, the final x_A starts to increase until the new steady state is reached. On the other hand, decreasing the split fraction causes the final mole fraction to initially increase and then decrease back until a new steady state is reached. A lower split fraction results in a higher flowrate entering the bottom CSTR causing a lower residence time with a higher initial rate of change in the bottom CSTR (increasing x_A) accounting for the early spike of x_{Af}. As the top CSTR catches up, the overall conversion decreases until the new steady state is reached.

v) Since all responses reach a steady state value, this indicates that the poles of the transfer models are all negative and on the left-hand side of the S-plane (real poles). The shape of the response is of an "S" shape when examining x_{At}, x_{Ab} and x_{Af}, which suggests that the transfer model from these variables to alpha is likely to be a second order function with 2 real poles.

vi) Although the system is non-linear, the time constant does not vary considerably when the magnitude of the step input changes from 0.5 to 0.55 compared to 0.5 to 0.9, however, the gain does vary significantly. As a result, the extent of non-linear behaviour does vary substantially because of the high variance of the gain as the step input changes to higher ranged values.

Alpha from 0.5 to 0.55

Par	Known	Value
K	☐	0.025063
Tp1	☐	0.95238
Tp2	☐	0.52632

Alpha from 0.5 to 0.65

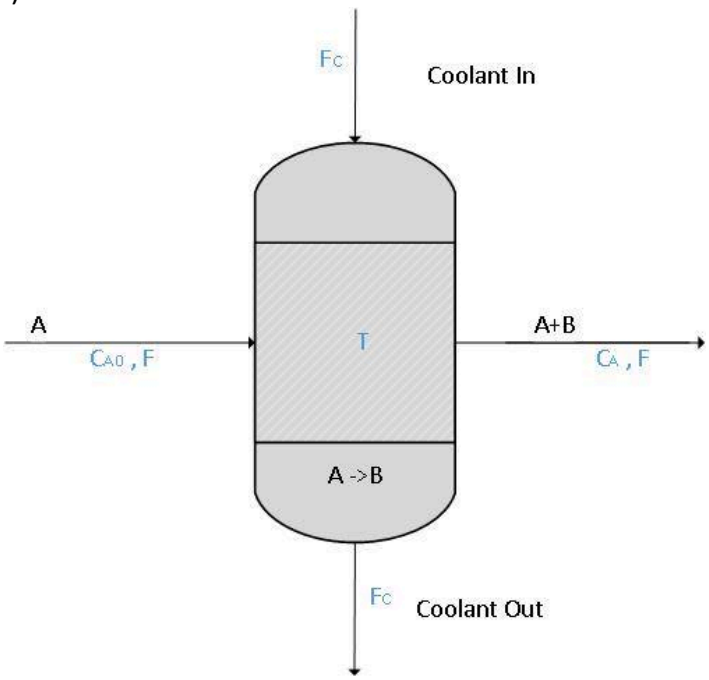
Par	Known	Value
K	☐	0.076726
Tp1	☐	0.86957
Tp2	☐	0.58824

Alpha from 0.5 to 0.95

Par	Known	Value
K	☐	0.28213
Tp1	☐	0.90909
Tp2	☐	0.68966

Portfolio 3

i)



ii)

Material balance on component A

$$V\frac{dc_A}{dt} = F(c_{Ao} - c_A) - Vk_o e^{-\frac{E}{RT}} c_A$$

Energy balance

$$V\rho c_p \frac{dT}{dt} = F\rho c_p (T_o - T) - \frac{aF_c^{b+1}}{F_c + \frac{aF_c^b}{2\rho_c c_{pc}}}(T - T_c) + (-\Delta H_{rxn})Vk_o e^{-\frac{E}{RT}} c_A$$

Assumptions:

- Well mixed, constant volume CSTR
- Liquid only
- Constant volumetric feed flowrate

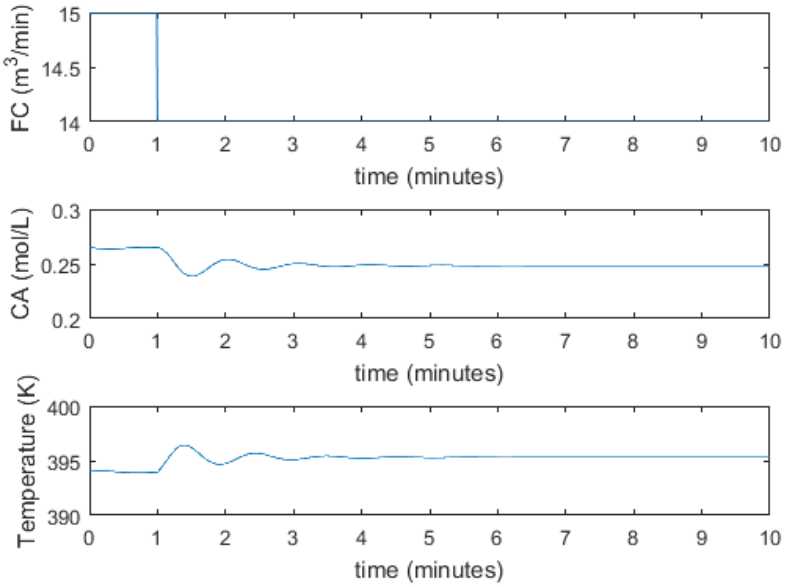
Steady State Values:
T = 393.9521 K C_A = 0.2646 mol/L
See Appendix B for MATLAB script used to determine these values.

$F=1m^3/min$
$V=1m^3$
$C_{A0}=2kmol/m^3$
$T_0=323K$
$c_p=1cal/(g*K)$
rho-$10^6 g/m^3$
$k_0=1*10^{10}min^{-1}$

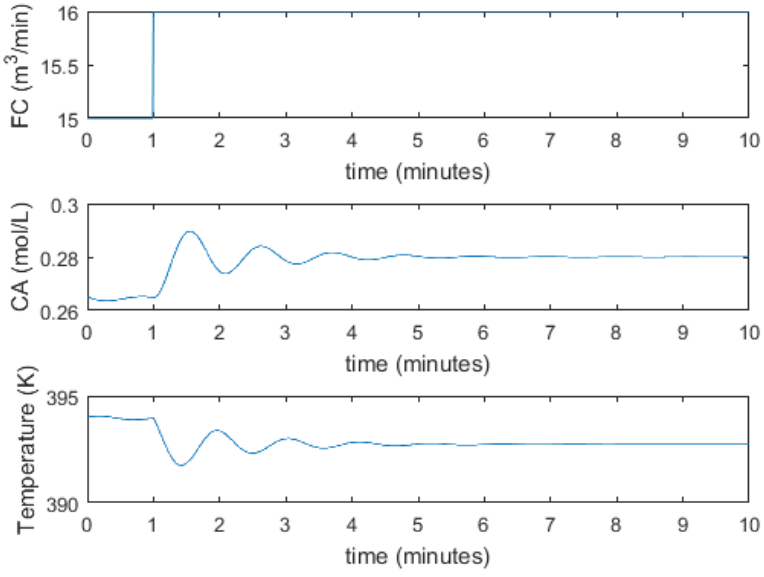
$E/R=8330.1$ K
$-\Delta H_{rxn} = 130 \times 10^6$ cal/kmol
$T_C=365K$ $F_{C,ss}=15$ m^3/min
$C_{pc}=1$ cal/(g*K)
$rho_C=1 \times 10^6$ g/m^3
$a = 1.678x10^6$ cal/(min*K)
$b=0.5$

iii)

Coolant Flowrate step down 1 m^3/min from 15 m^3/min to 14 m^3/min



Coolant Flowrate step up 1 m^3/min from 15 m^3/min to 16 m^3/min



iv)

The reduction in coolant flow rate begins to increase the reactor temperature until a new steady-state is achieved. This exothermic reaction adds heat to the system and a reduction in cooling (decrease in coolant flow rate) with relatively constant heat production from the reaction means the temperature will increase as the amount of heat being removed decreases but the amount being added remains relatively constant. An increase in temperature means an increase in reaction rate and conversion as indicated by Arrhenius' law. Therefore, less cooling, which produces a higher steady-state temperature will result in higher conversion of A and therefore, a lower concentration of it leaving the reactor. Conversely, more cooling will result in lower temperatures, a lower conversion of A and a higher concentration of A leaving the reactor.

v) The oscillating shape of the responses tell us that the transfer models for both dependent variables are underdamped. They reach steady-state values indicating that the roots to the transfer models are all negative on the real axis. When examining the response in CA, there is more of an "S" shape at the initiation of the step than in the response in T. This suggests that the transfer model from C_A to F_C is likely a relative second order function and since we know an underdamped function requires two poles(making it second order), this transfer function must have 2 poles with no numerator dynamics or 3 poles with one zero. On the other hand, the response in T appears to be first-order, indicating it's transfer function is 2^{nd} order underdamped with 1 zero which gives a relative order of 1.

vi) This system is rather non-linear as all parts of the transfer function (gain, taus and zeta) vary considerably when the magnitude of the step input changes. As shown in appendix C, a step change of 5 m^3/minute in the coolant flow rate produced very different transfer model parameters (gain, taus, zeta) whereas the step size of 1 or 2 m^3/min produced transfer function models that were more similar to each other.

Appendix A – Portfolio 1 MATLAB Code and Steady-State Data

```
Fo = 1; %moles/time
F5 = 1.7; % moles/time
xia = 0.95;
tau = 1/2.7; % time
F3 = 1.8; % moles/time
ko = 2.7; % 1/time
M = 1;
F1 = Fo+F5;

xiss = 0.95;
R = F3/F1^2/F5*(F1+ko*M);
x1ss = -R*Fo*xia/(1-R*F1); %2/3
x2ss = x1ss*F1/(F1+ko*M); %1/3
x3ss = F1*x2ss/F3; %1/2

%% No Time Delay - Recycle and non-Recycle
figure(1)
subplot(4, 1, 1)
plot(tout, xi+xiss, 'r-')
hold on
plot(tout, xi_0+xiss, 'b--')
title('xi')
legend('Recycle', 'Non-Recycle')
subplot(4, 1, 2)
plot(tout, x1+x1ss, 'r-')
hold on
plot(tout, x1_0+x1ss, 'b--')
title('x1')
legend('Recycle', 'Non-Recycle')
subplot(4, 1, 3)
plot(tout, x2+x2ss, 'r-')
hold on
plot(tout, x2_0+x2ss, 'b--')
title('x2')
legend('Recycle', 'Non-Recycle')
subplot(4, 1, 4)
plot(tout, x3+x3ss, 'r-')
hold on
plot(tout, x3_0+x3ss, 'b--')
title('x3')
legend('Recycle', 'Non-Recycle')
```

Appendix B - Portfolio3, MATLAB script to determine Steady-State values

```
F = 1;
V = 1;
cao = 2;
To = 323;
cp = 1;
rho = 1E6;
ko = 1E10;
ER = 8330.1;
negH = 130E6;
Tc = 365;
Fcss = 15;
cpc = 1;
rhoc = 1E6;
a = 1.678E6;
b = 0.5;

dcdt = @(x) [F*(cao-x(1)) - V*ko*exp(-ER/x(2))*x(1)];
dTdt = @(x) [F*rho*cp*(To - x(2)) +
a*Fcss^(b+1)/(Fcss+a*Fcss^b/(2*rhoc*cpc))*(Tc - x(2)) + negH*V*ko*exp(-
ER/x(2))*x(1)];

x0 = [0.265, 394];
solvethis = @(x) [dcdt(x) dTdt(x)];

real_roots = fsolve(solvethis, x0)
```

Appendix C – system ID transfer model estimator parameters for various step inputs
Using 3 poles, underdamped and zero, the following estimates were obtained

Input (coolant flow rate)(m^3/min): 15 to 14 15 to 13 15 to 10

Temperature:

Par	Known	Value
K	☐	-1.3493
Tw	☐	0.16363
Zeta	☐	0.16817
Tp3	☐	0.0063394
Tz	☐	0.13921
Td	☐	0

Par	Known	Value
K	☐	-1.4253
Tw	☐	0.15957
Zeta	☐	0.19403
Tp3	☐	0.013911
Tz	☐	0.14667
Td	☐	0

Par	Known	Value
K	☐	-1.7183
Tw	☐	0.14185
Zeta	☐	0.34376
Tp3	☐	0.054163
Tz	☐	0.19338
Td	☐	0

C_A:

Par	Known	Value
K	☐	0.016158
Tw	☐	0.16357
Zeta	☐	0.16824
Tp3	☐	0.10493
Tz	☐	0.11008
Td	☐	0

Par	Known	Value
K	☐	0.016491
Tw	☐	0.15937
Zeta	☐	0.193
Tp3	☐	0.11043
Tz	☐	0.11968
Td	☐	0

Par	Known	Value
K	☐	0.01752
Tw	☐	0.14043
Zeta	☐	0.31605
Tp3	☐	0.20481
Tz	☐	0.22346
Td	☐	0