Problem statement : (Example 2.1 from Process Dynamics and Control, Third edition)

EXAMPLE 2.1

A stirred-tank blending process with a constant liquid holdup of 2 m^3 is used to blend two streams whose densities are both approximately 900 kg/m^3. The density does not change during mixing.

(a) Assume that the process has been operating for a long period of time with flow rates of $w_1 = 500$ kg/min and $w_2 =$ 200 kg/min, and feed compositions (mass fractions) of $x_1 = 0.4$ and $x_2 = 0.75$. What is the steady-state value of x?

(b) Suppose that w_1 changes suddenly from 500 to 400 kg/min and remains at the new value. Determine an expression for $x(t)$ and plot it.

(c) Repeat part **(b)** for the case where w_2 (instead of w_1) changes suddenly from 200 to 100 kg/min and remains there.

(d) Repeat part **(c)** for the case where x_1 suddenly changes from 0.4 to 0.6.

(e) For parts **(b)** through **(d)**, plot the normalized response $x_N(t)$,

$$x_N(t) = \frac{x(t) - x(0)}{x(\infty) - x(0)}$$

where $x(0)$ is the initial steady-state value of $x(t)$ and $x(\infty)$ represents the final steady-state value, which is different for each part.

$$\frac{dV}{dt} = \frac{1}{\rho}(w_1 + w_2 - w) \qquad (2\text{-}17)$$

$$\frac{dx}{dt} = \frac{w_1}{V\rho}(x_1 - x) + \frac{w_2}{V\rho}(x_2 - x) \qquad (2\text{-}18)$$

The dynamic model in Eqs. 2-17 and 2-18 is quite general and is based on only two assumptions: perfect mixing and constant density. For special situations, the liquid volume V is constant (that is, $dV/dt = 0$), and

Method 1 for solving the same question.

```
%% Example 2.1 A stirred tank blending process  page No.19
%% for Case (a) w1=500/400 w2=200;
%%          (b) w1=500, w2=200/100
%%          (c) w1=500, w2=100, x2=0.4/0.6
V=2;           %liquid holdup Volume(m3)
w1=500;w2=200; % Stream flow rates (Kg/min) w1,w2;
x1=.6;x2=.75;  %feed composition(mass fraction) x1, x2;
w=w1+w2;       % total flow rate (Kg/min);
d=900;         % density of fluids, constant for both streams
tou=(V*d)/w;   % liquid holdup time
v=[w1 x1 w2 x2 w tou];
tspan=[0 25];  % time period(min)
x0=0.5;        % Initialization x(0)=0.5;
[t,x]=ode45(@calc,tspan,x0); % Function calling
hold on
plot(t,x)
```

(2nd m-file for defining function)

```
function dx_dt=calc(t,x)
% r=[w1 x1 w2 x2 w tou];
V=2; %liquid holdup Volume(m3)
w1=500;w2=200; % Stream flow rates (Kg/min) w1,w2;
x1=.6;x2=.75; %feed composition(mass fraction) x1, x2;
w=w1+w2; % total flow rate (Kg/min);
d=900; % density of fluids, constant for both streams
tou=(V*d)/w; % liquid holdup time
v=[w1 x1 w2 x2 w tou];
r=v;
c=(((r(1)*r(2)+r(3)*r(4))/r(5)));
dx_dt=(c-x)/r(6);
end
```

Method 2 for solving the same question.

```
%% Example 2.1 A stirred tank blending process  page No.19
%% for Case (a) w1=500 to 400 w2=200; (b) w1=500, w2=200 to 100 (c) w1=500, w2=100, ↙
x2=0.4 to 0.6
V=2; %liquid holdup Volume(m3)
w1=500;w2=200; % Stream flow rates (Kg/min) w1,w2;
x1=.6;x2=.75; %feed composition(mass fraction) x1, x2;
w=w1+w2; % total flow rate (Kg/min);
d=900; % density of fluids, constant for both streams
tou=(V*d)/w; % liquid holdup time
v=[w1 x1 w2 x2 w tou];
tspan=[0 25];% time period(min)
x0=0.5;% Initialization x(0)=0.5;
[t,x]=ode45(@(t,x)calc(t,x,v),tspan,x0); % Function calling
hold on
plot(t,x)

function dx_dt=calc(t,x,r)
% r=[w1 x1 w2 x2 w tou];
c=(((r(1)*r(2)+r(3)*r(4))/r(5)));
dx_dt=(c-x)/r(6);

end
```

Problem statement : (Example 2.5 from Process Dynamics and Control, Third edition)

EXAMPLE 2.5

To illustrate how the CSTR can exhibit nonlinear dynamic behavior, we simulate the effect of a step change in the coolant temperature T_c in positive and negative directions. Table 2.3 shows the parameters and nominal operating

Table 2.3 Nominal Operating Conditions for the CSTR

Parameter	Value	Parameter	Value
q	100 L/min	E/R	8750 K
c_{Ai}	1 mol/L	k_0	7.2×10^{10} min^{-1}
T_i	350 K	UA	5×10^4 J/min K
V	100 L	$T_c(0)$	300 K
ρ	1000 g/L	$c_A(0)$	0.5 mol/L
C	0.239 J/g K	$T(0)$	350 K
$-\Delta H_R$	5×10^4 J/mol		

condition for the CSTR based on Eqs. 2–66 and 2–68 for the exothermic, irreversible first-order reaction A → B. The two-state variables of the ODEs are the concentration of A (c_A) and the reactor temperature T. The manipulated variable is the jacket water temperature, T_c.

Two cases are simulated, one based on increased cooling by changing T_c from 300 K to 290 K and one reducing the cooling rate by increasing T_c from 300 K to 305 K.

These model equations are solved in MATLAB with a numerical integrator (ode15s) over a 10 min horizon. The decrease in T_c results in an increase in c_A. The results are displayed in two plots of the temperature and reactor concentration as a function of time (Figs. 2.7 and 2.8).

At a jacket temperature of 305 K, the reactor model has an oscillatory response. The oscillations are characterized by apparent reaction run-away with a temperature spike. However, when the concentration drops to a low value, the reactor then cools until the concentration builds, then there is

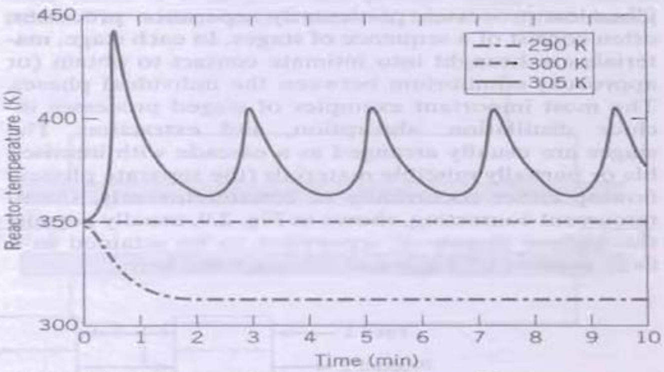

Figure 2.7 Reactor temperature variation with step changes in cooling water temperature from 300 K to 305 K and from 300 K to 290 K.

For the stated assumptions, the unsteady-state component balances for species A (in molar units) is

$$V\frac{dc_A}{dt} = q(c_{Ai} - c_A) - Vkc_A \qquad (2\text{-}66)$$

The following form of the CSTR energy balance is convenient for analysis and can be derived from Eqs. 2-62 and 2-63 and Assumptions 1–8 (Fogler, 2006; Russell and Denn, 1972),

$$V\rho C\frac{dT}{dt} = wC(T_i - T) + (-\Delta H_R)Vkc_A + UA(T_c - T) \qquad (2\text{-}68)$$

```
% main file where ODE is executed with plots to get the final results
clc
close all;
Q=100;
Cai=1;
Ti=350;
V=100;
rho=1000;
C=0.239;
delHr=50000;
ebyr=8750;
ko=7.2*10^10;
UtimesA=50000;
Tco=305;
t=[0 10];
tf=10;
X0=[0.50 350.0];
% next command solves ODE by calling test function
[t,X] = ode15s(@test,t,X0);
figure
plot(t(:,1),X(:,1));
figure
plot(t(:,1),X(:,2));


function [ Xdot ] = test(t,X )
Q=100;
Cai=1;
Ti=350;
V=100;
rho=1000;
C=0.239;
delHr=50000;
ebyr=8750;
ko=7.2e10;
UtimesA=50000;
Tco=305;
% calculation of w is tricky as its not given in direct form
W=1e5;
% F=[Q*(Cai-X(1))/V-ko*exp(-ebyr*(1/X(2))*X(1));...
%     (W*(Ti-X(2)))/(rho*C)+(delHr*ko*exp(-
ebyr*(1/X(2))*X(1)))/(rho*C)+UA*(Tco-X(2))/(V*rho*C)];
Xdot= [Q*(Cai-X(1))/V-ko*exp(-ebyr*(1/X(2)))*X(1);...
    (W*(Ti-X(2)))/(rho*V)+(delHr*ko*exp(-
ebyr*(1/X(2)))*X(1))/(rho*C)+UtimesA*(Tco-X(2))/(V*rho*C)];
end
```