Assumption

- Product B is produced and reactant A is consumed in each of the three perfectly mixed reactors
- by a **first-order reaction** occurring in the liquid.
- both temperatures and the liquid volumes are assumed to be constant
- Density is assumed constant throughout the system
- If the volume and density of each tank are constant, the total mass in each tank is constant

SERIES OF ISOTHERMAL,CONSTANT-HOLDUP CSTRs

Single CSTR Problem

$$A \overset{k}{\rightarrow} B$$

$$\text{Flow of A into system} = F_0 C_{A0}$$

$$\text{Flow of A out of system} = F C_A$$

$$\text{Rate of formation of A from reaction} = -VkC_A$$

$$\text{Time rate of change of A inside tank} = \frac{d(VC_A)}{dt}$$

Total Mass Balance

$$\frac{d(\rho V)}{dt} = F_0 \rho_0 - F\rho$$

Balance Around for **component A**

$$\frac{d(VC_A)}{dt} = F_0 C_{A0} - FC_A - VkC_A$$

Similarly Component B

$$\frac{d(VC_B)}{dt} = F_0 C_{B0} - FC_B + VkC_A$$

Total Continuity Equation

$$\frac{d(\rho V_1)}{dt} = \rho F_0 - \rho F_1 = 0$$

The total mass in each tank is constant(Constant Holdup).

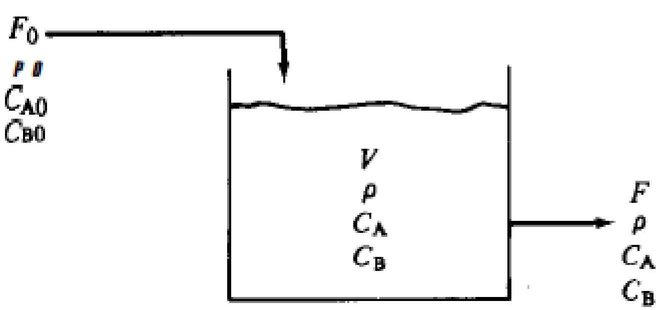
$F_3=F_2=F_1=F_0=F$

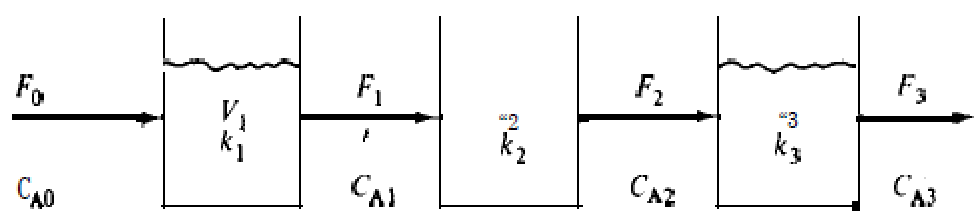
For Component A

$$V_1 \frac{dC_{A1}}{dt} = F(C_{A0} - C_{A1}) - V_1 k_1 C_{A1}$$

$$V_2 \frac{dC_{A2}}{dt} = F(C_{A1} - C_{A2}) - V_2 k_2 C_{A2}$$

$$V_3 \frac{dC_{A3}}{dt} = F(C_{A2} - C_{A3}) - V_3 k_3 C_{A3}$$





SERIES OF ISOTHERMAL,CONSTANT-HOLDUP CSTRs

Total Continuity Equation

$$\frac{d(\rho V_1)}{dt} = \rho F_0 - \rho F_1 = 0$$

The total mass in each tank is constant(Constant Holdup).

$F_3=F_2=F_1=F_0=F$

For Component A

$$V_1 \frac{dC_{A1}}{dt} = F(C_{A0} - C_{A1}) - V_1 k_1 C_{A1}$$

$$V_2 \frac{dC_{A2}}{dt} = F(C_{A1} - C_{A2}) - V_2 k_2 C_{A2}$$

$$V_3 \frac{dC_{A3}}{dt} = F(C_{A2} - C_{A3}) - V_3 k_3 C_{A3}$$

The flows are all equal to *F but can vary with time*

The parameters must be known

$V_1, V_2, V_3, k_1, k_2,$ and k_3

$$k_n = \alpha e^{-E/RT_n} \qquad n = 1, 2, 3$$

$$\frac{dC_{A1}}{dt} + \left(k + \frac{1}{\tau}\right)C_{A1} = \frac{1}{\tau} C_{A0}$$

$$\frac{dC_{A2}}{dt} + \left(k + \frac{1}{\tau}\right)C_{A2} = \frac{1}{\tau} C_{A1}$$

$$\frac{dC_{A3}}{dt} + \left(k + \frac{1}{\tau}\right)C_{A3} = \frac{1}{\tau} C_{A2}$$

where $\tau = V/F$

one forcing function or input variable, C_{A0}

three unknowns or dependent variables: C_{A1}, C_{A2}, and C_{A3}

CSTRs WITH VARIABLE HOLDUPS

Reactor 1: $\frac{dV_1}{dt} = F_0 - F_1$

$$\frac{d}{dt}(V_1 C_{A1}) = F_0 C_{A0} - F_1 C_{A1} - V_1 k_1(C_{A1})$$

Reactor 2: $\frac{dV_2}{dt} = F_1 - F_2$

$$\frac{d}{dt}(V_2 C_{A2}) = F_1 C_{A1} - F_2 C_{A2} - V_2 k_2(C_{A2})$$

Reactor 3: $\frac{dV_3}{dt} = F_2 - F_3$

$$\frac{d}{dt}(V_3 C_{A3}) = F_2 C_{A2} - F_3 C_{A3} - V_3 k_3(C_{A3})$$

six first-order nonlinear ordinary differential equations

k_1, k_2, k_3 and n parameter

CA1, CA2, CA3, *VI, V2, and V,*
$C_{A0(t)}$ and $F_{0(t)}$

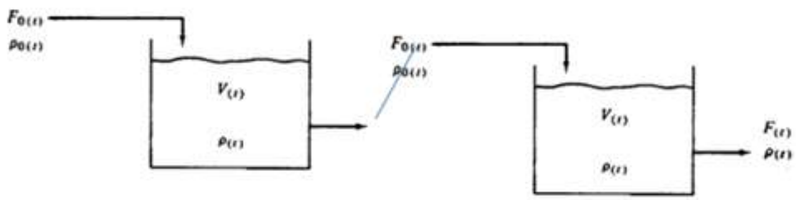
Degrees of freedom
6 equation
9 variables

$C_{A1}, C_{A2}, C_{A3}, V_1, V_2, V_3, F_1, F_2,$ and F_3.

Level of the control valve

$F_1 = f_{(V_1)}$ $F_2 = f_{(V_2)}$ $F_3 = f_{(V_3)}$

TWO HEATED TANKS



$$\frac{d(\rho V_1)}{dt} = \rho F_0 - \rho F_1 = 0$$

- Density ρ constant
- Volumes V constant
- heat capacities Cp constant

$$F_0 = F_1 = F_2 = F$$

1

$$F_0 \rho_0 (U_0 + K_0 + \phi_0) - F\rho(U + K + \phi) + (Q_G + Q)$$
$$- (W + FP - F_0 P_0) = \frac{d}{dt}[(U + K + \phi)V\rho]$$

$$\frac{d(\rho V U)}{dt} = F_0 \rho_0 U_0 - F\rho U + Q_G + Q - F\rho \frac{P}{\rho} + F_0 \rho_0 \frac{P_0}{\rho_0}$$
$$= F_0 \rho_0 (U_0 + P_0 \bar{V}_0) - F\rho(U + P\bar{V}) + Q_G + Q$$

$$\frac{d(\rho V U)}{dt} = F_0 \rho_0 h_0 - F\rho h + Q - \lambda V k C_A \qquad \left(H \text{ or } h \equiv U + P\bar{V} \right)$$

$$h = C_p T \qquad \rho C_p \frac{d(VT)}{dt} = \rho C_p (F_0 T_0 - FT) + Q - \lambda V k C_A$$

Energy balance around Tank 1

$$\frac{d(\rho C_p V_1 T_1)}{dt} = \rho C_p (F_0 T_0 - F_1 T_1) + Q_1$$

Energy balance around Tank 1

$$\frac{d(\rho C_p V_2 T_2)}{dt} = \rho C_p (F_1 T_1 - F_2 T_2)$$

- **Density ρ constant**
- **Volumes V constant**
- **heat capacities Cp constant**

$$\rho C_p V_1 \frac{dT_1}{dt} = \rho C_p F(T_0 - T_1) + Q_1$$

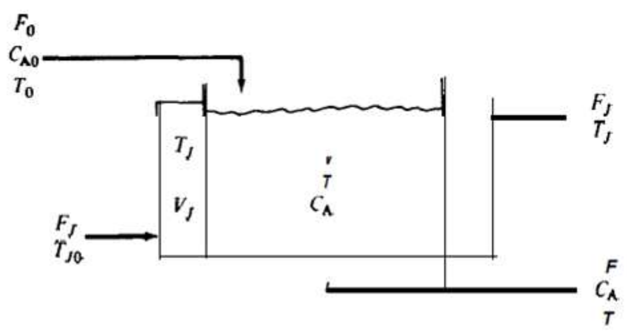
$$\rho C_p V_2 \frac{dT_2}{dt} = \rho C_p F(T_1 - T_2)$$

Degrees of Freedom

ρ, Cp, V_1, V_2, , and F is Parameter of the Model or specified

Heat input to the first tank Q_1 need to be specified

NONISOTHERMAL CSTR (PERFECTLY MIXED COOLING JACKET)



$$A \xrightarrow{k} B$$

Reactor total continuity:

$$\frac{dV}{dt} = F_0 - F$$

Reactor component A continuity:

$$\frac{d(VC_A)}{dt} = F_0\, C_{A0} - FC_A - Vk(C_A)$$

Reactor energy equation :

$$\rho\,\frac{d(Vh)}{dt} = \rho(F_0\, h_0 - Fh) - \lambda V k (C_A)^n - UA_H(T - T_J)$$

Cooling Jacket heat transfer $Q = UA_H(T - T_J)$

Jacket Energy Equation

$$\rho_J\, V_J\, \frac{dh_J}{dt} = F_J\, \rho_J (h_{J0} - h_J) + UA_H(T - T_J)$$

Hydraulic- between reactor holdup and the flow out of the reactor

$$F = K_V(V - V_{min})$$

$$\frac{dV}{dt} = F_0 - F$$

$$\frac{d(VC_A)}{dt} = F_0\, C_{A0} - FC_A - V(C_A)^n \alpha e^{-E/RT}$$

$$\rho C_p\, \frac{d(VT)}{d\ t} = \rho C_p (F_0\, T_0 - FT) - \lambda V (C_A)^n \alpha e^{-E/RT} - UA_H(T - T_J)$$

$$\rho_J\, V_J C_J\, \frac{dT_J}{dt} = F_J\, \rho_J\, C_J (T_{J0} - T_J) + UA_H(T - T_J)$$

$$F = K_V(V - V_{min})$$

Degrees of freedom: V, F, C_A, T and T_J

Initial Condition: T_0, F_0, C_{A0} AND F_J

Parameters need to be defined

n, a, E, R, p, $C_{,,}$ U, $A_{,,}$ ρ_J, $V_{,,}$ C_J, T_{J0}, K_V, and V_{min}

SERIES OF ISOTHERMAL,CONSTANT-HOLDUP CSTRs

Total Continuity Equation

$$\frac{d(\rho V_1)}{dt} = \rho F_0 - \rho F_1 = 0$$

The total mass in each tank is constant(Constant Holdup).

$F_3=F_2=F_1=F_0=F$

For Component A

$$V_1 \frac{dC_{A1}}{dt} = F(C_{A0} - C_{A1}) - V_1 k_1 C_{A1}$$

$$V_2 \frac{dC_{A2}}{dt} = F(C_{A1} - C_{A2}) - V_2 k_2 C_{A2}$$

$$V_3 \frac{dC_{A3}}{dt} = F(C_{A2} - C_{A3}) - V_3 k_3 C_{A3}$$

The flows are all equal to *F but can vary with time*

The parameters must be known

$V_1, V_2, V_3, k_1, k_2,$ and k_3

$$k_n = \alpha e^{-E/RT_n} \qquad n = 1, 2, 3$$

$$\frac{dC_{A1}}{dt} + \left(k + \frac{1}{\tau}\right)C_{A1} = \frac{1}{\tau} C_{A0}$$

$$\frac{dC_{A2}}{dt} + \left(k + \frac{1}{\tau}\right)C_{A2} = \frac{1}{\tau} C_{A1}$$

$$\frac{dC_{A3}}{dt} + \left(k + \frac{1}{\tau}\right)C_{A3} = \frac{1}{\tau} C_{A2}$$

where $\tau = V/F$

one forcing function or input variable, C_{A0}

three unknowns or dependent variables: C_{A1}, C_{A2}, and C_{A3}

$$\frac{dC_{A1}}{dt} = \frac{1}{\tau_1}(C_{A0} - C_{A1}) - k_1 C_{A1}$$

$$\frac{dC_{A2}}{dt} = \frac{1}{\tau_2}(C_{A1} - C_{A2}) - k_2 C_{A2} \qquad \tau_i = V_i / F$$

$$\frac{dC_{A3}}{dt} = \frac{1}{\tau_3}(C_{A2} - C_{A3}) - k_3 C_{A3}$$

$$C_{Am} = C_{Am}^{ss} + K_c \left[e(t) + \frac{1}{\tau_I} \int_0^t e(\xi) d\xi \right]$$

$$C_{A0} = C_{Ad} + C_{Am}$$

$$e(t) = C_{A3}^{sp} - C_{A3}$$

```
DECLARE
  TYPE
    Concentration  = 0.1 :   0.0 :  100    UNIT = 'kmol/m3'
    Conc_diff      =   0 :  -100 :  100    UNIT = 'kmol/m3'
    Rate           =   0 :  -1E9 :  1E9    UNIT = 'kmol/(m3 h)'
END
```

```
# ---------- CSTR ------------------
MODEL CSTR

PARAMETER
  Tau, k              AS REAL

VARIABLE
  Ca, Ca_In, Ca_out AS Concentration

EQUATION

  $Ca = (Ca_In - Ca) / tau - k * Ca;
  Ca_out = Ca;

END # CSTR

# ------------ PI -------------------
MODEL PI

PARAMETER
  Kc, Ti              AS REAL

VARIABLE
  Cm, Cmss, Set_point AS Concentration
  e                   AS Conc_diff
  w                   AS Rate

EQUATION

  Cm = Cmss + Kc * (e + w / Ti);
  $w = e;

END # PI
```

```
# ------------ TRAIN -----------------
MODEL TRAIN

UNIT
  CSTR1           AS CSTR
  CSTR2           AS CSTR
  CSTR3           AS CSTR
  CONTROLLER      AS PI

VARIABLE
  Ca_d            AS Concentration

SET
  CSTR1.tau := 2;
  CSTR2.tau := 2;
  CSTR3.tau := 2;
  CSTR1.k := 0.5;
  CSTR2.k := 0.5;
  CSTR3.k := 0.5;
  CONTROLLER.Kc := 10;
  CONTROLLER.Ti := 4;

EQUATION
  CONTROLLER.Cm + Ca_d = CSTR1.Ca_in;
  CSTR1.Ca_out = CSTR2.Ca_in;
  CSTR2.Ca_out = CSTR3.Ca_in;
  CONTROLLER.e = CONTROLLER.Set_point
               - CSTR3.Ca_out;

END # TRAIN
```

```
PROCESS CSTR_Series

  UNIT
    Series   AS TRAIN

  ASSIGN
    WITHIN Series DO
      Ca_d                 := 0.4;
      CONTROLLER.Cmss      := 0.4;
      CONTROLLER.Set_point := 0.1;
    END

  INITIAL
    WITHIN Series DO
        CSTR1.Ca = 0.4;
        CSTR2.Ca = 0.2;
        CSTR3.Ca = 0.1;
        CONTROLLER.w = 0;
    END

  SCHEDULE
    SEQUENCE
      CONTINUE FOR 5
      RESET
        Series.Ca_d := 0.6;
      END
      CONTINUE FOR 45
      RESET
        Series.CONTROLLER.Set_point := 0.15;
      END
      CONTINUE FOR 50
    END
END
```

MATLAB script file

```
global Ca3sp Camss Kc taui Cad tau1 tau2 tau3 k1 k2 k3

tau1 = 2; tau2 = 2; tau3 = 2; taui = 4;
k1 = 0.5; k2 = 0.5; k3 = 0.5; Kc = 10;
Cad = 0.4; Ca3sp = 0.1; Camss = 0.4;

y0 = [0.4 0.2 0.1 0];  % initial condition
[t,y] = ode45('CSTR_series',[0 5],y0);
e = Ca3sp - y(:,3);
Cad = 0.6;              % disturbance at t = 5 h
[t1,y1] = ode45('CSTR_series',[5 50],y(end,:));
e1 = Ca3sp - y1(:,3);
Ca3sp = 0.15;           % setpoint change at t = 50 h
[t2,y2] = ode45('CSTR_series',[50 100],y1(end,:));
e2 = Ca3sp - y2(:,3);
t = [t;t1;t2];
y = [y;y1;y2];
e = [e;e1;e2];
Cam = Camss + Kc * (e + y(:,4)/taui);
plot(t,[y(:,1:3) Cam]);
legend('CA1','CA2','CA3','CAm');
ylabel('CA (kmol/m^3)'); xlabel('time (h)');
```

ODE file

```
function dy = CSTR_series(t,y)

global Ca3sp Camss Kc taui Cad ...
       tau1 tau2 tau3 k1 k2 k3

e = Ca3sp-y(3);
Cam = Camss+Kc*(e+y(4)/taui);
Cao = Cad+Cam;
dy = [(Cao-y(1))/tau1-k1*y(1);
      (y(1)-y(2))/tau2-k2*y(2);
      (y(2)-y(3))/tau3-k3*y(3);
      e];
```

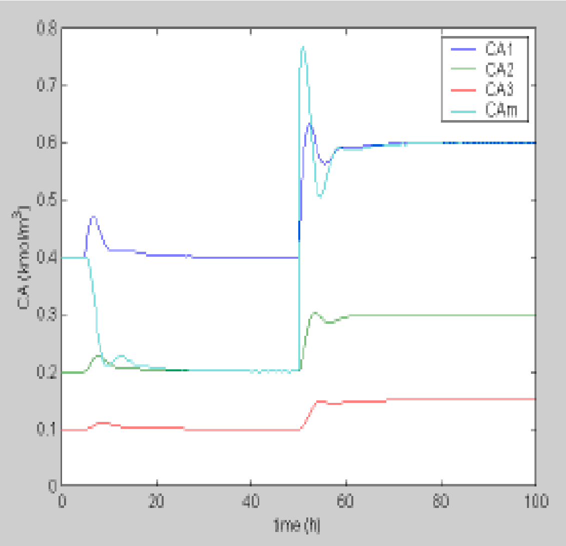


Table 2-2: Equation Solving

Type	Notation	Function
Linear Equations	, n equations, n variables	\ (slash)
Nonlinear Equation of One Variable		fzero
Nonlinear Equations	, n equations, n variables	fsolve

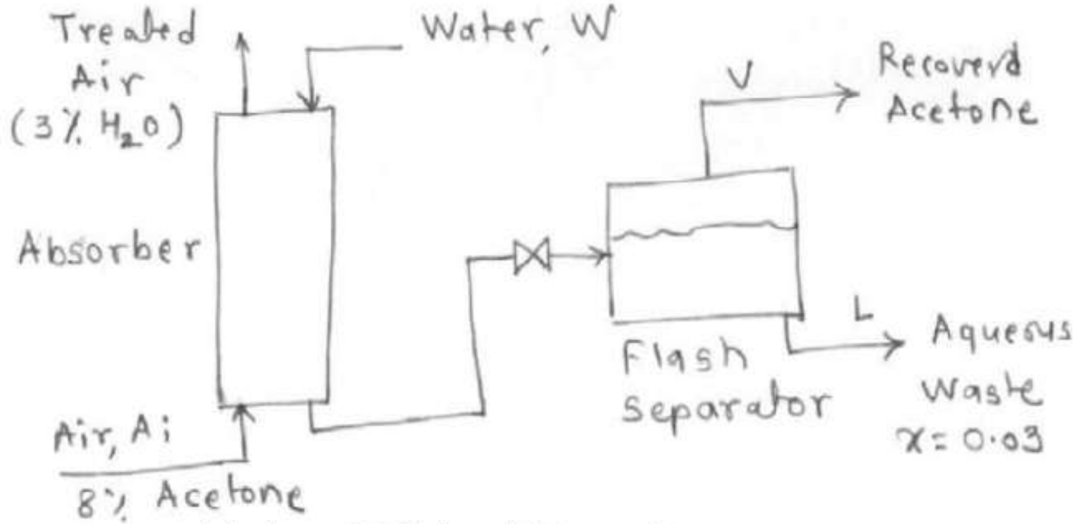
$$
\begin{aligned}
2x - 3y + 4z &= 5 \\
x + y + 4z &= 10 \\
3x + 4y - 2z &= 0
\end{aligned}
$$

C = [2,-3,4; 1,1,4; 3,4,-2], B = [5; 10; 0]

$$
: \begin{bmatrix} 2 & -3 & 4 \\ 1 & 1 & 4 \\ 4 & 4 & -2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 5 \\ 10 \\ 0 \end{bmatrix}
$$

A = C\B, x = A(1), y = A(2), z = A(3)

$$
\begin{aligned}
3x_1 + 11x_2 - 2x_3 &= 7 \\
x_1 + x_2 - 2x_3 &= 4 \\
x_1 - x_2 + x_3 &= 19
\end{aligned}
$$



Air in flow: 600 lb /hr with 8 mass % acetone
Water flow rate: 500 lb/hr

$$Air \quad : \quad 0.92Ai = 0.97Ao$$

$$Acetone \quad : \quad 0.08\,Ai = 0.03\,L + y\,V$$

$$Water \quad : \quad W = 0.03\,Ao + (1-y)V + 0.97L$$

$$Design\ requirement \quad : \quad x = 0.03$$

$$y = 20.5x$$

$$\begin{bmatrix} 0.97 & 0 & 0 \\ 0 & 0.03 & 0.615 \\ 0.03 & 0.385 & 0.97 \end{bmatrix} \begin{bmatrix} Ao \\ L \\ V \end{bmatrix} = \begin{bmatrix} 0.92 \times 600 \\ 0.08 \times 600 \\ 500 \end{bmatrix}$$

$$0 = C_H - C_{H_0} + \left(k_1 C_H^{1/2} C_M + k_2 C_H^{1/2} C_X\right)\tau$$

$$0 = C_M - C_{M_0} + k_1 C_H^{1/2} C_M \tau$$

$$0 = \left(k_1 C_H^{1/2} C_M + k_2 C_H^{1/2} C_X\right)\tau - C_X$$

$h = C_H$

$k_1 = 55.2$

$m = C_M$

$k_2 = 30.2$

$x = C_X$

$C_{H0} = .021$

$C_{M0} = .0105$

```
syms h m x;

eq1=h-.021+(55.2*m*h^0.5+30.2*x*h^0.5)*0.5;
eq2=m-0.0105+(55.2*m*h^0.5)*0.5;
eq3=(55.2*m*h^0.5-30.2*x*h^0.5)*0.5-x;
```

Step 2: Next, to solve this system of equations, we type

```
S=solve(eq1,eq2,eq3);
```

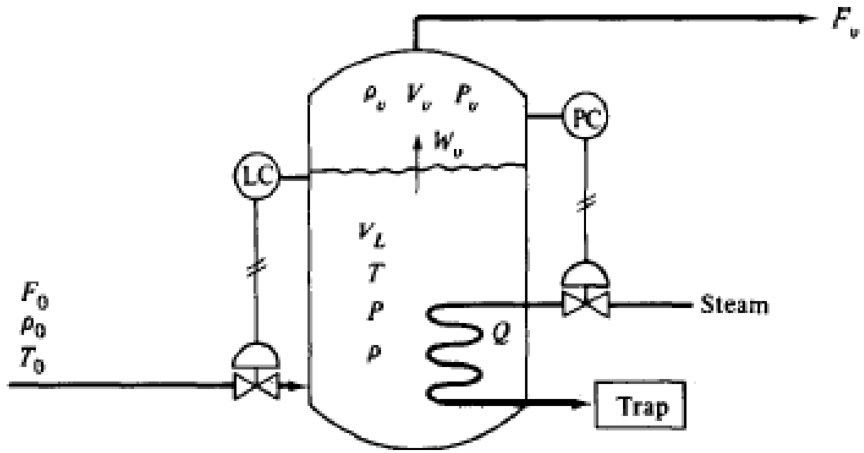
$$2x_1 - x_2 - e^{-x_1} = 0$$

$$-x_1 + 2x_2 - e^{-x_2} = 0,$$

starting at `x0 = [-5 -5]`.

```
function F = myfun(x)
F = [2*x(1) - x(2) - exp(-x(1));
      -x(1) + 2*x(2) - exp(-x(2))];
```

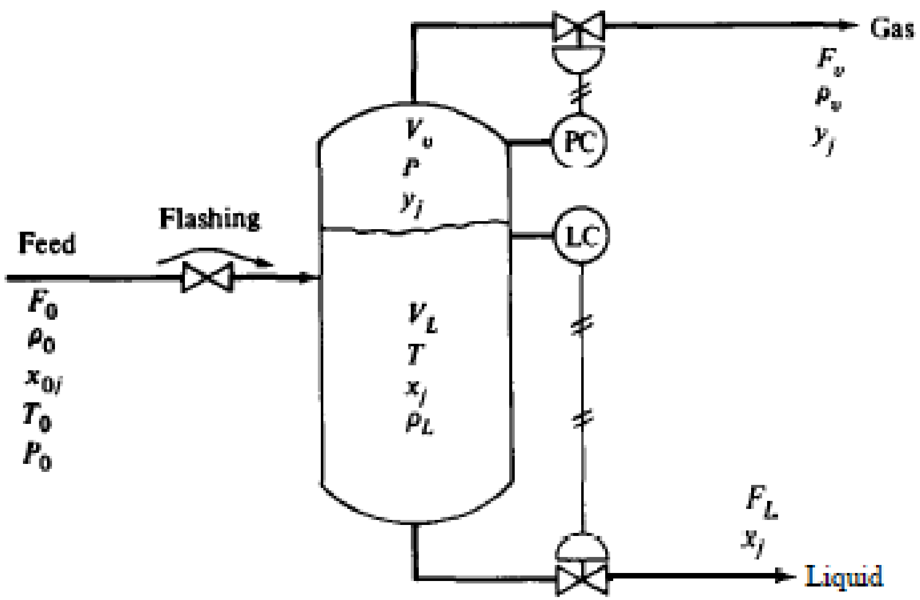
```
x0 = [-5; -5];                % Make a starting guess at the solution
options=optimset('Display','iter');   % Option to display output
[x,fval] = fsolve(@myfun,x0,options)  % Call optimizer
```



$$\rho_v F_v (H_v - h_0) = Q$$

where H_v = enthalpy of vapor leaving tank (Btu/lb_m or cal/g)

h_0 = enthalpy of liquid feed (Btu/lb_m or cal/g)



Gas
F_v
ρ_v
y_j
V_v
P
y_j
PC
LC
Flashing
Feed
F_0
ρ_0
x_{0j}
T_0
P_0
V_L
T
x_j
ρ_L
F_L
x_j
Liquid

$\rho_L = f_{(x_j, T)}$ (3.48) $\rho_v = \frac{M_v^{av} P}{R\,T}$ (3.49)

average molecular weight

$$M_v^{av} = \sum_{j=1}^{NC} M_j y_j$$

Total continuity:

$$\rho_0 F_0 = \rho_v F_v + \rho_L F_L \qquad (3.51)$$

Component continuity:

$$\frac{\rho_0 F_0}{M_0^{av}} x_{0j} = \frac{\rho_v F_v}{M_v^{av}} y_j + \frac{\rho_L F_L}{M_L^{av}} x_j \qquad (3.52)$$

Vapor-liquid equilibrium :

$$y_j = f_{(x_j, T, P)} \qquad (3.53)$$

Energy equation :

$$h_0 \rho_0 F_0 = H \rho_v F_v + h \rho_L F_L \qquad (3.54)$$

Thermal properties :

$$h_0 = f_{(x_{0j}, T_0)} \qquad h = f_{(x_j, T)} \qquad H = f_{(y_j, T, P)}$$

The number of variables in the system $9 + 2(NC - 1)$:

$\rho_v, F_v, M_v^{av}, y_1, y_2, \ldots, y_{NC-1}, \rho_L, F_L, M_L^{av}, x_1, x_2, \ldots, x_{NC-1}, T, h$, and H.

Pressure P and all the feed properties are given.

	Equation	Number of equations
Total continuity	(3.51)	1
Energy	(3.54)	1
Component continuity	(3.52)	NC-1
Vapor-liquid equilibrium	(3.53)	NC
Densities of vapor and liquid	(3.48) and (3.49)	2
Thermal properties for liquid and vapor streams	(3.55)	2
Average molecular weights	(3.50)	2
		$2NC + 7$