Chapter 22

22.1

Microwave Operating States

Condition	Fan	Light	Timer	Rotating Base	Microwave Generator	Door Switch
Open the door Place the food inside	OFF	ON	OFF	OFF	OFF	ON
Close the door	OFF	OFF	OFF	OFF	OFF	OFF
Set the time	OFF	OFF	OFF	OFF	OFF	OFF
Heat up food	ON	ON	ON	ON	ON	OFF
Cooking complete	OFF	OFF	OFF	OFF	OFF	OFF

Safety Issues:

- Door switch is always OFF before the microwave generator is turned ON.
- Fan always ON when microwave generator is ON.

22.2

Input Variables:

ON
STOP
EMERGENCY

Output Variables:

START (1)
STOP (0)

Truth Table

ON	STOP	EMERGENCY	START/STOP
1	1	1	0
0	1	1	0
1	0	1	0
0	0	1	0
1	1	0	0
0	1	0	0
1	0	0	1
0	0	0	0

The truth state table is used to find the logic law that relates inputs with outputs:

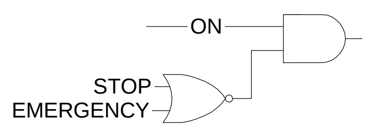
$$ON \bullet \overline{STOP} \bullet \overline{EMERGENCY}$$

Applying Boolean Algebra we can obtain an equivalent expression:

$$ON \bullet (\overline{STOP} \bullet \overline{EMERGENCY}) = ON \bullet (\overline{STOP + EMERGENCY})$$

Finally the binary logic and ladder logic diagrams are given in Figure S22.2:

<u>Binary Logic Diagram:</u>



<u>Ladder Logic Diagram</u>

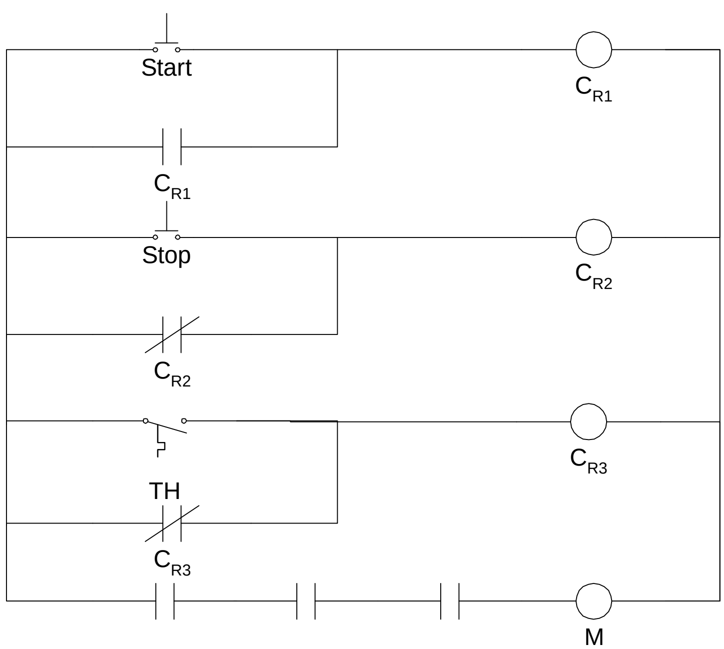


Figure S22.2.

22.3

A	B	Y
0	0	1
1	0	1
0	1	0
1	1	1

From the truth table it is possible to find the logic operation that gives the desired result,

$$\overline{\overline{A} \bullet B}$$

Since a NAND gate is equivalent to an OR gate with two negated inputs, our expression reduces to: $\overline{\overline{A} \bullet B} = A + \overline{B}$

Finally the binary logic diagram is given in Figure S22.3.

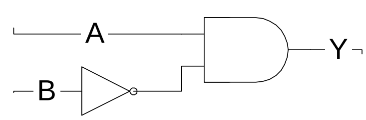
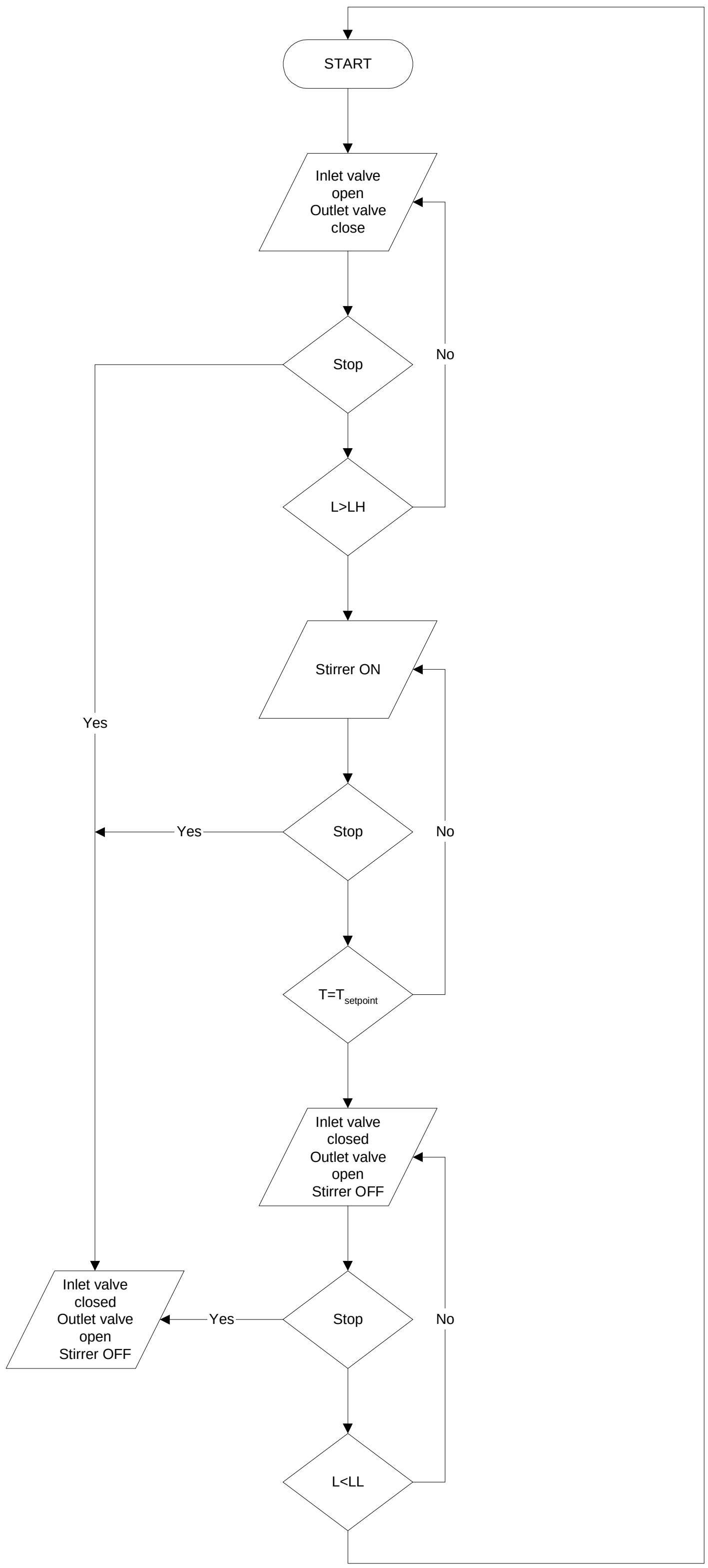


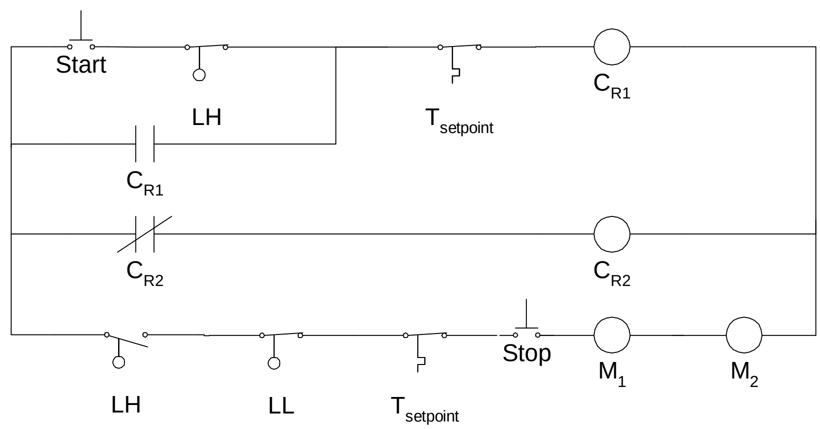
Figure S22.3.

22.4

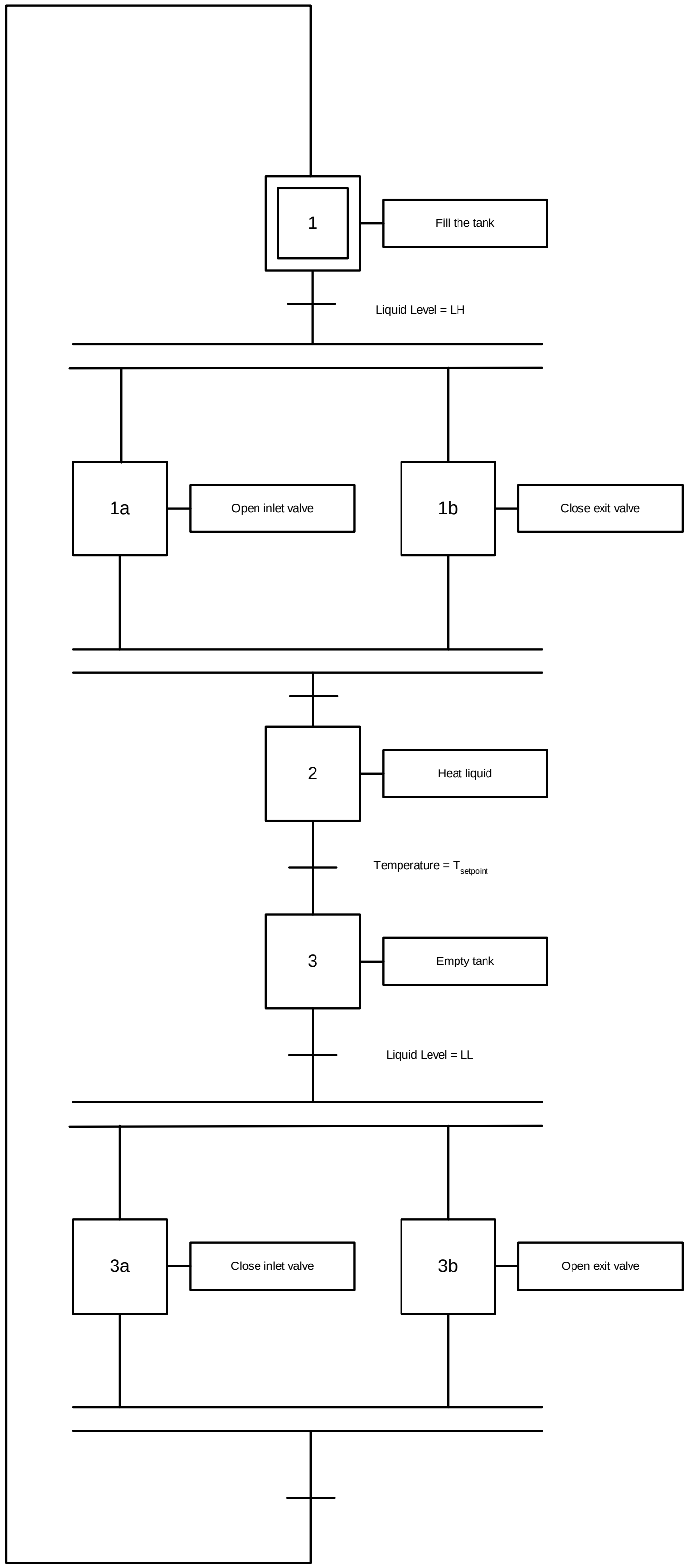
Information Flow Diagram



Ladder Logic Diagram



Sequential Function Chart

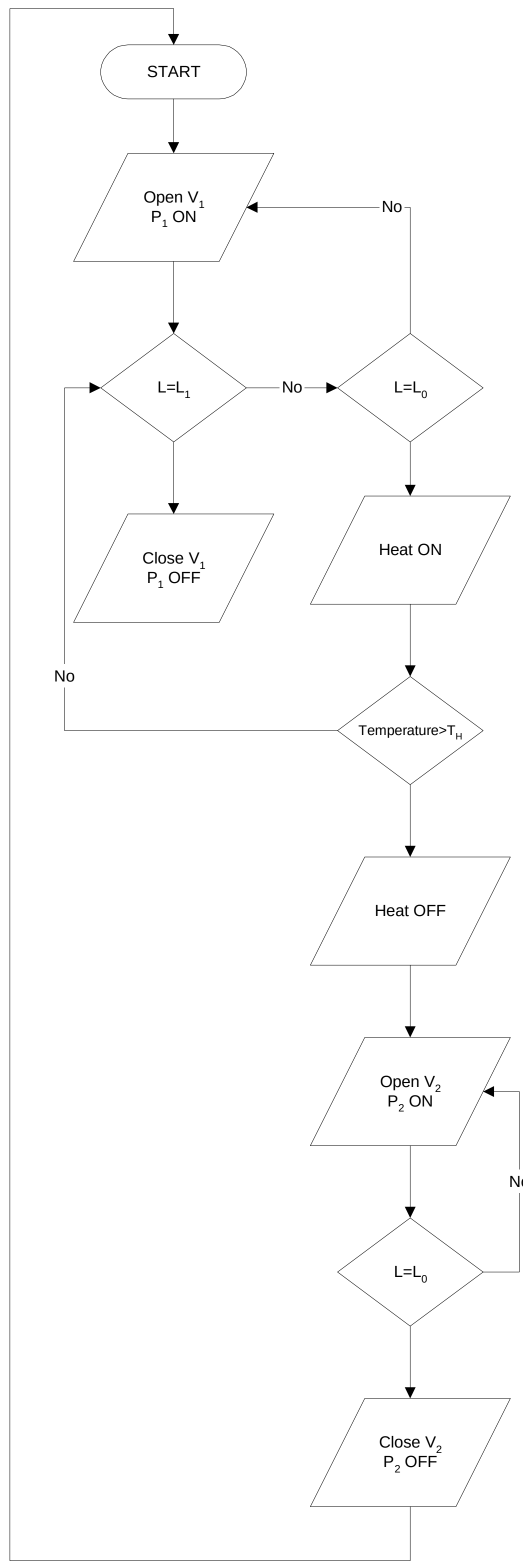


1
Fill the tank
Liquid Level = LH
1a
Open inlet valve
1b
Close exit valve
2
Heat liquid
Temperature = T setpoint
3
Empty tank
Liquid Level = LL
3a
Close inlet valve
3b
Open exit valve

Figure S22.4.

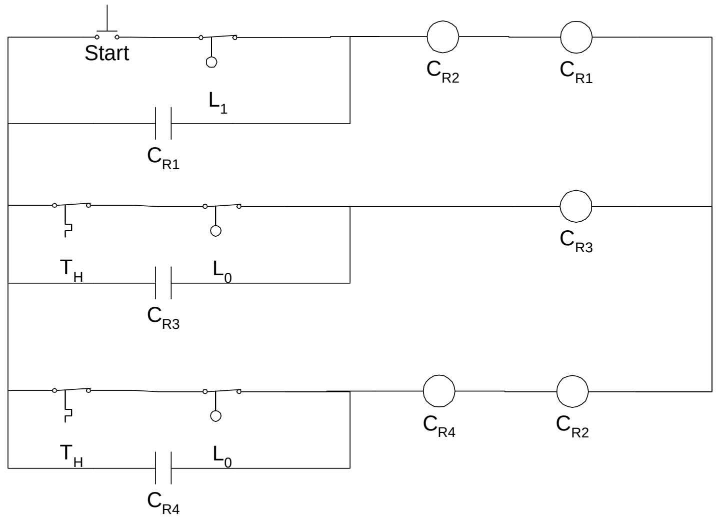
22.5

Information Flow Diagram



Ladder Logic Diagram:

R1= Pump 1   R2= Valve 2   R3= Heater   R4= Pump 2



Sequential Function Chart:

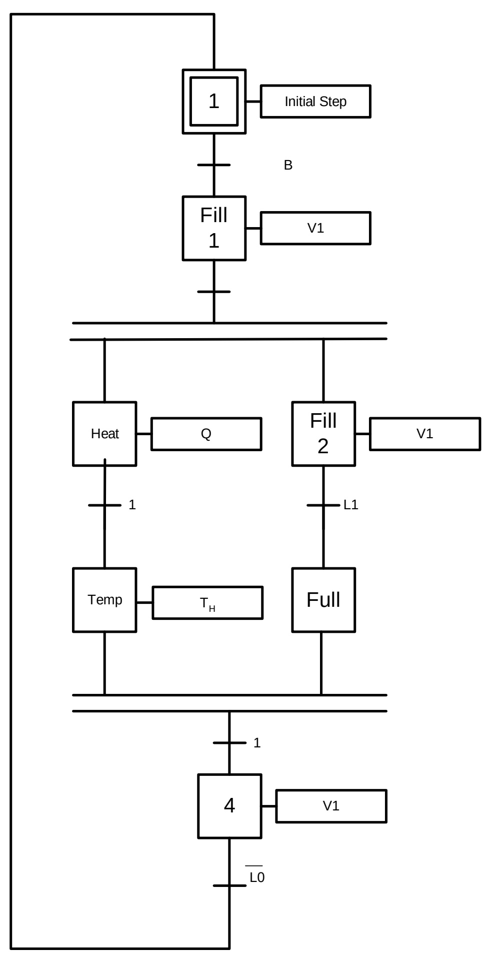
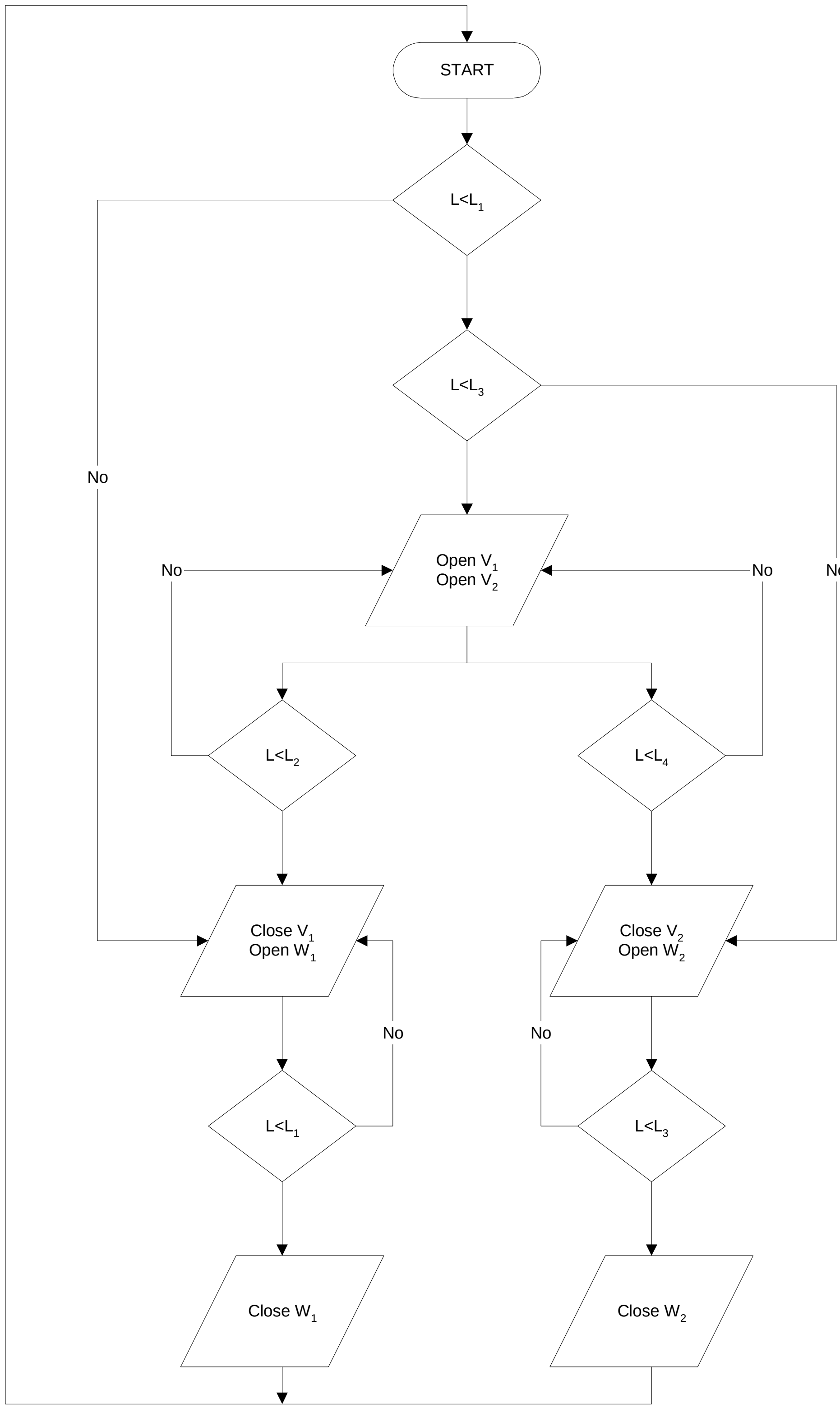


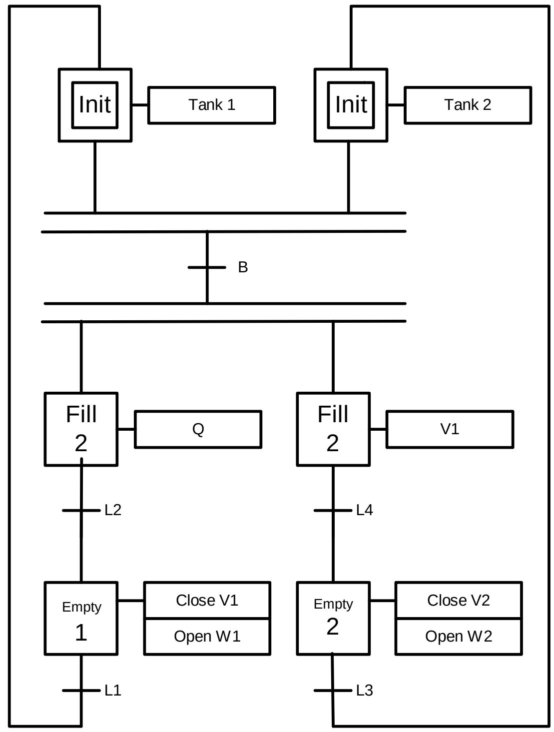
Figure S22.5.

22.6

Information Flow Diagram:



Sequential Function Chart:



Ladder Logic Diagram:

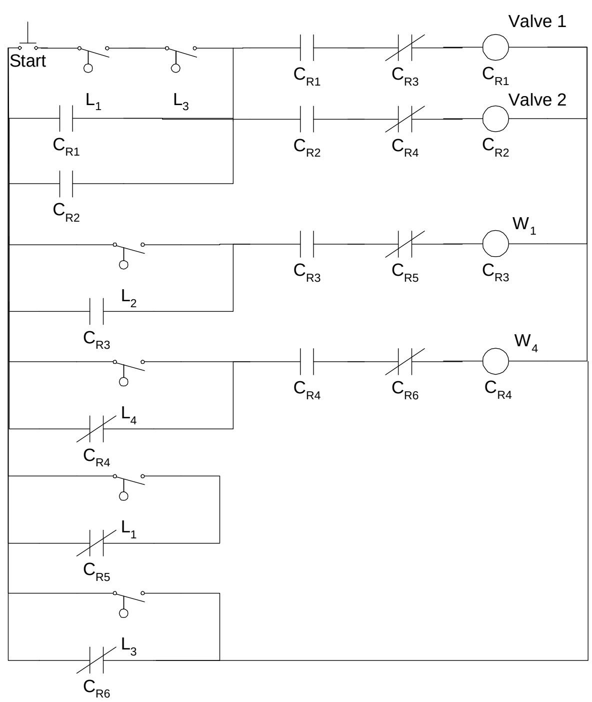
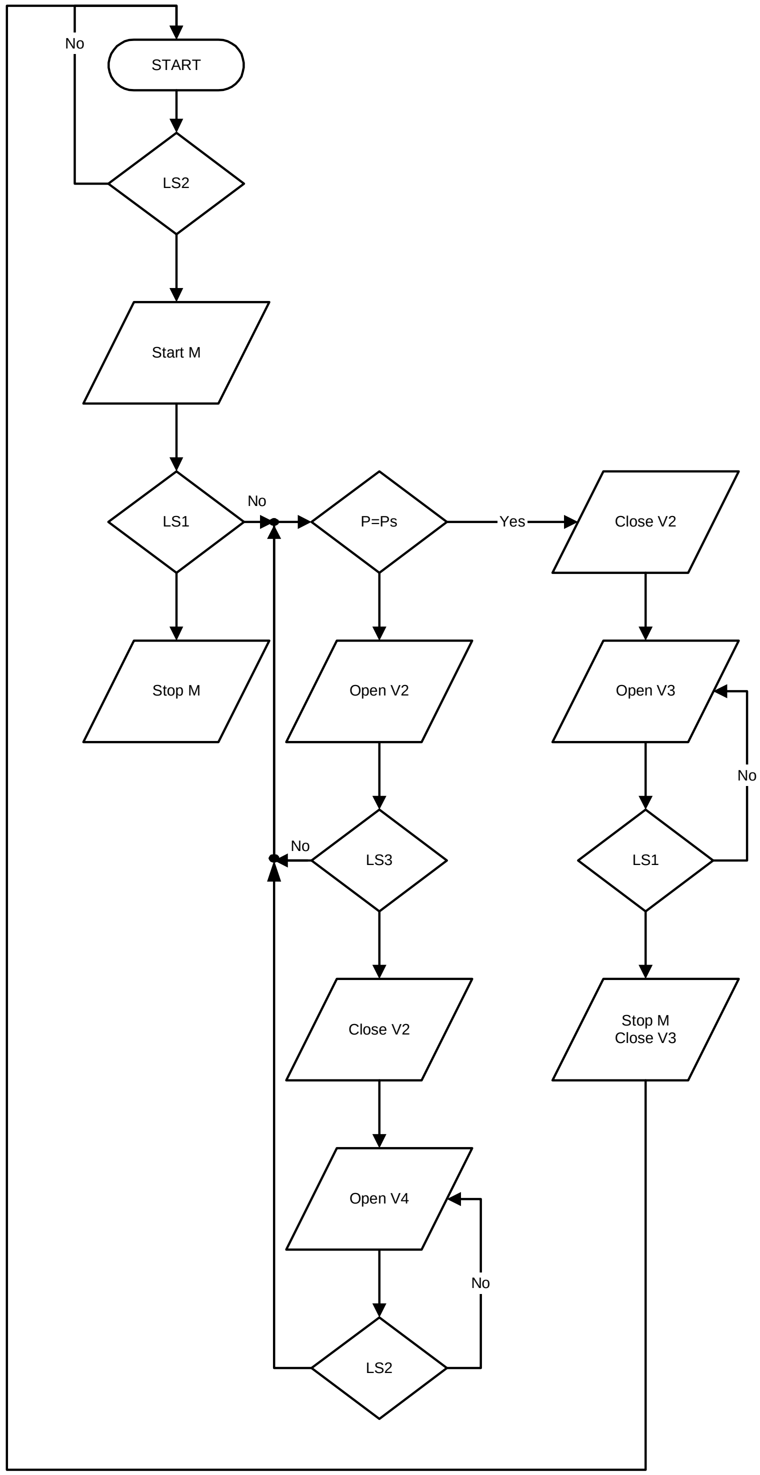


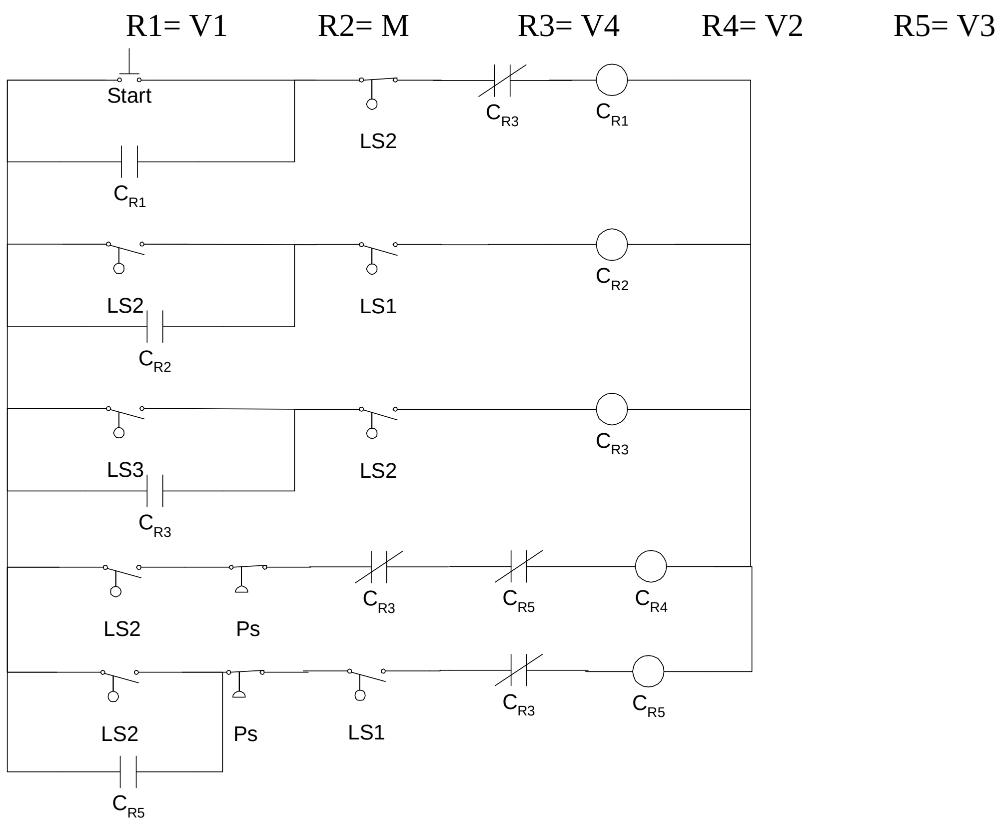
Figure S22.6.

22.7

Information Diagram:



Ladder Logic Diagram:



Sequential Function Chart:

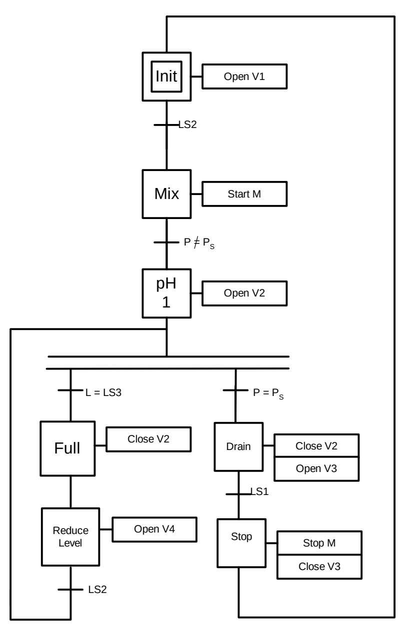


Figure S22.7.

22.8

In batch processing, a sequence of one or more steps is performed in a defined order, yielding a finished product of a specific quantity. Equipment must be properly configured in unit operations in order to be operated and maintained in a reasonable manner.

The discrete steps necessary to carry out this operation could be:

.- Open exit valve in tank car.

.- Turn on pump 1

.- Empty the tank car by using the pump and transfer the chemical to the storage tank (assume the storage tank has larger capacity than the tank car)

.- Turn off pump 1

.- Close tank car valve (to prevent backup from storage tank)

.- Open exit valve in storage tank.

.- Transfer the chemical to the reactor by using the second pump

.- Close the storage tank exit valve and turn off pump 2.

.- Wait for the reaction to reach completion.

.- Open the exit valve in the reactor.

.- Discharge the resulting product

Safety concerns:

Because a hazardous chemical is to be handled, several safety issues must be considered:

.- Careful and appropriate transportation of the chemical, based on safety regulation for that type of product.

.- Appropriate instrumentation must also be used. Liquid level indicators could be installed so that pumps are turned off based on level.

.- Chemical leak testing, detection, and emergency shut-down

.- Emergency escape plan.

Therefore, care should be exercised when transporting and operating hazardous chemicals. First of all, tanks and units should be vented prior to charging. Generally, materials should be stored in a cool dry, well-ventilated location with low fire risk. In addition, outside storage tanks must be located at minimum distances from property lines.

Pressure, level, flow and temperature control could be utilized in all units. Hence, they must be equipped with instrumentation to monitor these variables. For instance, tank levels can be measured accurately with a float-type device, and storage temperatures could be maintained with external heating pads operated by steam or electricity. It is possible for a leak to develop between the tank car and storage tank, which could cause high flow rates, so a flow rate upper limit may be desirable.

Valves and piping should have standard connections. Enough valves are required to control flow under normal and emergency conditions. Centrifugal pumps are often preferred for most hazardous chemicals. In any case, the material of construction must take into account product chemical properties.

Don't forget that batch process control often requires a considerable amount of logic and sequencing for their operation. Besides, interlocks and overrides are usually considered to analyze and treat possible failure modes.

22.9

1.- Because there is no steady state for a batch reactor, a new linearization point is selected at t = 0. Then,

Linearization point for batch reactor: $t = 0 \;\; \equiv t^*$

2.- Available information:

$$k = 2.4\times10^{15}e^{-20000/T}\,(\text{min}^{-1}) \quad \text{where } T \text{ is in } {}^{\text{o}}\text{R}$$

$$C = 0.843\frac{\text{BTU}}{\text{lb}^{\text{o}}\text{F}} \qquad V = 1336\ \text{ft}^3$$

$$\rho = 52\frac{\text{lb}}{\text{ft}^3} \qquad q = 26\frac{\text{ft}^3}{\text{min}}$$

$$(-\Delta H) = 500\frac{\text{kJ}}{\text{mol}} \qquad C_{Ai} = 0.8\frac{\text{mol}}{\text{ft}^3}$$

$$T_i = 150^{\text{o}}\,\text{F} \qquad T_s = 25^{\text{o}}\,\text{C}$$

$$UA = 142.03\frac{\text{kJ}}{\text{min}^{\text{o}}\text{F}}$$

For continuous reactor, $\bar{T} = 150^{\text{o}}\,\text{F}$

Physical properties are assumed constant.

Problem solution:

A stirred batch reactor has the following material and energy balance equations:

$$-kC_A = \frac{dC_A}{dt} \tag{1}$$

$$(-\Delta H)kVC_A + UA(T_s - T) = V\rho C\frac{dT}{dt} \tag{2}$$

where $k = k_0 e^{-E/RT}$

From Eqs. 1 and 2, linearization gives:

$$-\left[k^{*}C_A{}^{*}+k^{*}C_A'+C_A{}^{*}k_0e^{-E/RT^{*}}\frac{E}{RT^{*2}}T'\right]=\frac{dC_A'}{dt} \tag{3}$$

$$(-\Delta H)V\left[k^{*}C_A{}^{*}+k^{*}C_A'+C_A{}^{*}k_0e^{-E/RT^{*}}\frac{E}{RT^{*2}}T'\right]$$

$$+UA(T_s'-T')=V\rho C\frac{dT'}{dt} \tag{4}$$

Rearranging, the following equations are obtained:

$$b_{11}C_A'+b_{12}T'=\frac{dC_A'}{dt} \tag{5}$$

$$b_{21}C_A+b_{22}T'+b_{23}T_s'=\frac{dT'}{dt} \tag{6}$$

where

$$b_{11}=-k_0e^{-E/RT^{*}}=-13.615$$

$$b_{12}=-k_0e^{-E/RT^{*}}C_A{}^{*}\left(\frac{E}{RT^{*2}}\right)=-0.586$$

$$b_{21}=\frac{(-\Delta H)k_0e^{-E/RT^{*}}}{\rho C}=155.30$$

$$b_{22}=\frac{1}{\rho C}(-\Delta H)k_0e^{-E/RT^{*}}C_A{}^{*}\left(\frac{E}{RT^{*2}}\right)-\frac{UA}{\rho VC}=6.66$$

$$b_{23}=\frac{UA}{\rho VC}=2.43\times10^{-3}$$

From Example 4.8, substituting values for continuous reactor

$$a_{11}=-13.636$$

$$a_{12}=-8.35\times10^{-4}$$

$$a_{21}=155.27$$

$$a_{22} = -0.0159$$

$$b_2 = 2.43\times 10^{-3}$$

(Note that , from material balance, $\bar{C}_A = 0.00114$)

Hence the transfer functions relating the steam jacket temperature $T_s'(s)$ and the tank outlet concentration $C_A'(s)$ are:

<u>Continuous reactor</u>:

$$\frac{C_A'(s)}{T_s'(s)} = \frac{-2.03\times 10^{-6}}{s^2 + 13.651s + 0.3464} = \frac{-5.86\times 10^{-6}}{2.887s^2 + 39.4s + 1}$$

then $\tau_{dom} \approx 35\,\text{min}$

<u>Batch reactor</u>:

$$\frac{C_A'(s)}{T_s'(s)} = \frac{-1.424\times 10^{-3}}{s^2 + 6.931s + 0.26} = \frac{-5.47\times 10^{-3}}{3.84s^2 + 26.65s + 1}$$

then $\tau_{dom} \approx 25\,\text{min}$

As noted in transfer functions above, the time constant for the batch is smaller than the time constant for the continuous reactor, but the gain is much larger.

22.10

The reactor equations are:

$$\frac{dx_1}{dt} = -k_1 x_1 \qquad (1)$$

$$\frac{dx_2}{dt} = k_1 x_1 - k_2 x_2 \qquad (2)$$

where $k_1 = 1.335\times10^{10} e^{-75,000/(8.31\times T)}$ and $k_2 = 1.149\times10^{17} e^{-125,000/(8.31\times T)}$

By using MATLAB, this differential equation system can be solved using the command "*ode45*". Furthermore we need to apply the command "*fminsearch*" in order to optimize the temperature. In doing so, the results are:

a) Isothermal operation to maximize conversion ($x_2(8)$):

$$T_{op} = 357.8 \text{ K} \quad \text{and} \quad x_{2max} = 0.3627$$

b) Cubic temperature profile: the values of the parameters in $T=a_0 + a_1 t + a_2 t^2 + a_3 t^3$ that maximize $x_2(8)$ are:

$$\begin{cases} a_0 = 372.78 \\ a_1 = -10.44 \\ a_2 = 2.0217 \\ a_3 = -0.1316 \end{cases} \quad \text{and} \quad x_{2max} = 0.3699$$

The optimum temperature profile and the optimum isothermal operation are shown in Fig. S22.10.

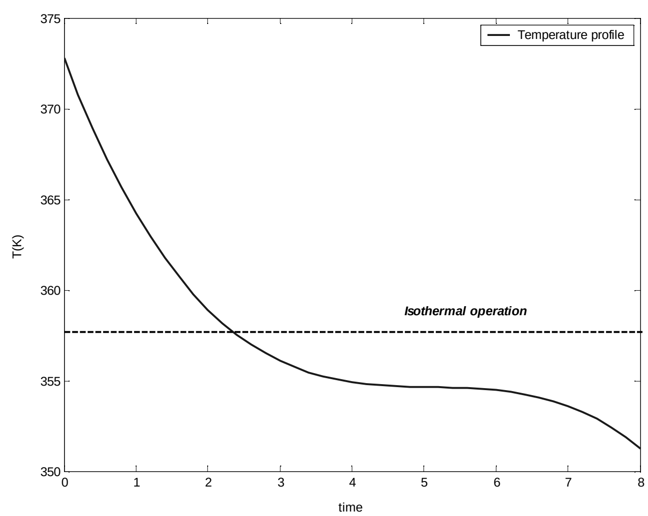


Figure S22.10. *Optimum temperature for the batch reactor.*

MATLAB simulation:

a) Constant temperature (First declare **Temp** as global variable)

1.- Define the differential equation system in a file called **batchreactor**.

```
function dx_dt=batchreactor(time_row,x)
global Temp
dx_dt(1,1)=-1.335e10*x(1)*exp(-75000/8.31/Temp);
dx_dt(2,1)=1.335e10*x(1)*exp(-75000/8.31/Temp) -
1.149e17*x(2)*exp(-125000/8.31/Temp);
```

2.- Define a function called **conversion** that gives the final value of x_2 (given a value of the temperature)

```
function x2=conversion(T)
global Temp
Temp=T;
x_0=[0.7,0];
[time_row, x] = ode45('batchreactor', [0 8], x_0 );
x2=-(x(length(x),2));
```

3.- Find the optimum temperature by using the command fminsearch

```
[T,negative_x2max]=fminsearch('conversion', To)
```

where T_o is our initial value to find the optimum temperature.

b) Temperature profile (First declare **a0 a1 a2 a3** as global variables)

1.- Define the differential equation system in a file called **batchreactor2**.

```
function dx_dt=batchreactor2(time_row,x)
global a0 a1 a2 a3
Temp=a0+a1*time_row+a2*time_row^2+a3*time_row^3;
dx_dt(1,1)=-1.335e10*x(1)*exp(-75000/8.31/Temp);
dx_dt(2,1)=1.335e10*x(1)*exp(-75000/8.31/Temp) -
1.149e17*x(2)*exp(-125000/8.31/Temp);
```

2.- Define a function called **conversion2** that gives the final value of x_2 (given the values of the temperature coefficients)

```
function x2b=conversion(a)
global a0 a1 a2 a3
a0=a(1);a1=a(2);a2=a(3);a3=a(4);x_0=[0.7,0];
[time_row, x] = ode45('batchreactor2', [0 8], x_0 );
x2b=-x(length(x),2);
```

3.- Find the optimum temperature profile by using the command fminserach

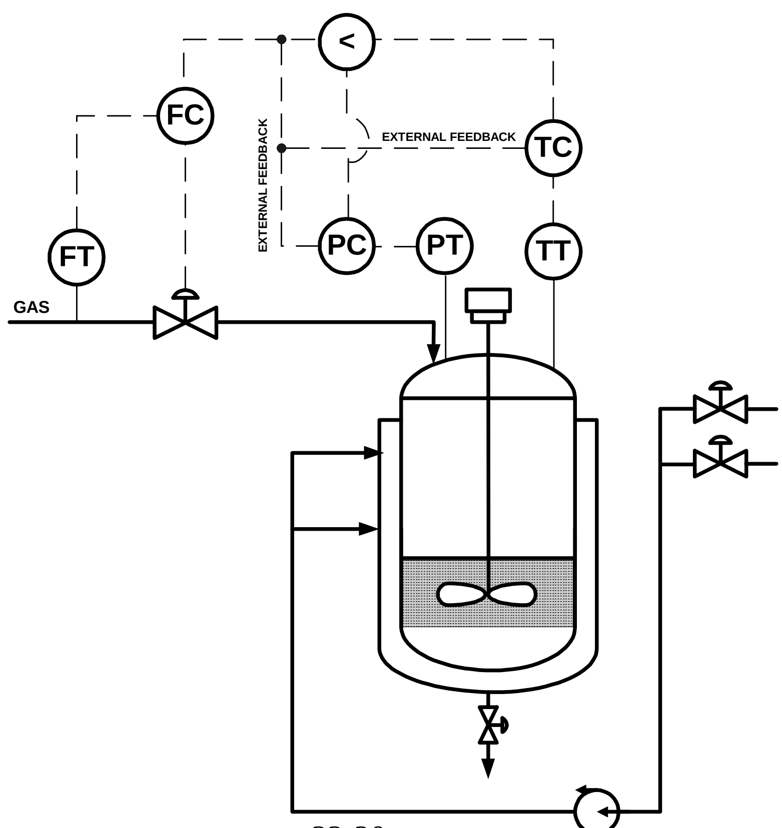
```
[T,negative_x2max]=fminsearch('conversion2', ao)
```

where a_o is the vector of initial values to find the optimum temperature profile.

22.11

The intention is to run the reactor at the maximum feed rate of the gas to minimize the time cycle, but the reactor is also cooling-limited. Therefore, if the pressure controller calls for a gas flow that exceeds the cooling capability of the reactor, the temperature will start to rise. The reaction temperature is not critical, but it must not exceed some maximum temperature. The temperature controller will then take over control of the feed valve and reduce the feed rate. The output of the selector sets the setpoint of a flow controller. The flow controller minimizes the effects of supply pressure changes on the gas flow rate. So this is a cascade type control system, with the primary controller being an override control system.

In an override control system, one of the controllers is always in a standby condition, which will cause that controller to saturate. Reset windup can be prevented by feeding back the selector relay output to the setpoint of each controller. Because the reset actions of both controllers have the same feedback signal, control will transfer when both controllers have no error. Then the outputs of both controllers will be equal to the signal in the reset sections. Because neither controller has any error, the outputs of both controllers will be the same. Particular attention must be paid to make sure that at least one controller in an override control system will always be in control. If not, then one of the controllers can wind up, and reset windup protection is necessary.



22.12

Material balance:

$$(-r_A) = -\frac{dC_A}{dt} = kC_{A0}{}^2(1-X)(\Theta_B - 2X)$$

Since

$$C_A = C_{A0}(1-X)$$

then

$$\frac{dX}{dt} = -\frac{1}{C_{A0}}\frac{dC_A}{dt}$$

Therefore

$$\boxed{\frac{dX}{dt} = kC_{A0}(1-X)(\Theta_B - 2X)} \qquad (1)$$

Energy balance:

$$\boxed{\frac{dT}{dt} = \frac{Q_g - Q_r}{NC_p}} \qquad (2)$$

where $Q_g = kC_{AO}{}^2(1-X)(\Theta_B - 2X)V(\Delta H_{RX})$
$Q_r = UA(T - 298)$

Eqs. 1 and 2 constitute a differential equation system. By using MATLAB, this system can be solved as long as the initial conditions are specified. Command "*ode45*" is suggested.

A.- ISOTHERMAL OPERATION UP TO 45 MINUTES

We will first carry out the reaction isothermally at 175 °C up to the time the cooling was turned off at 45 min.

Initial conditions : $X(0) = 0$ and $T(0) = 448$ K

Figure S22.12a shows the isothermal behavior for these first 45 minutes.

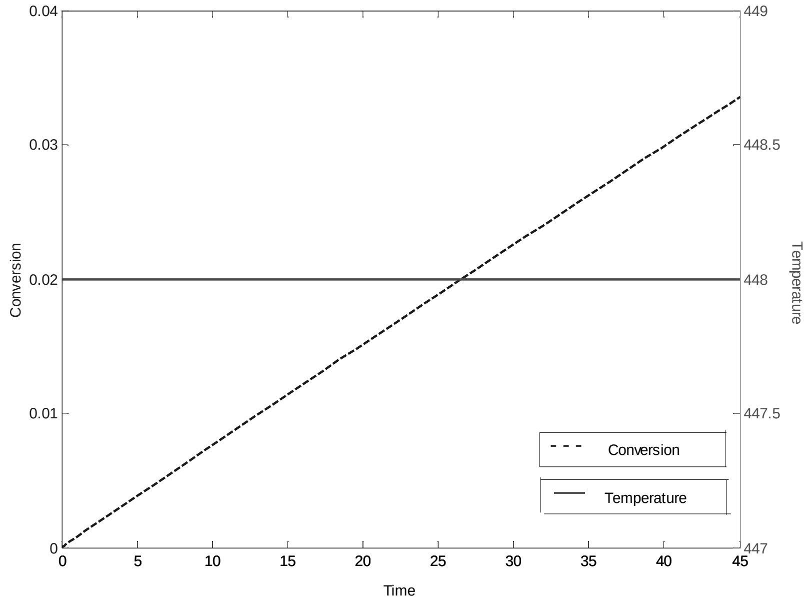


Figure S22.12a. *Isothermal behavior for the first 45 minutes*

B.- ADIABATIC OPERATION FOR 10 MINUTES

The cooling is turned off for 45 to 55 min. We will now use the conditions at the end of the period of isothermal operation as our initial conditions for adiabatic operation period between 45 and 55 minutes.

$$t = 45 \text{ min} \quad X = 0.033 \quad T = 448$$

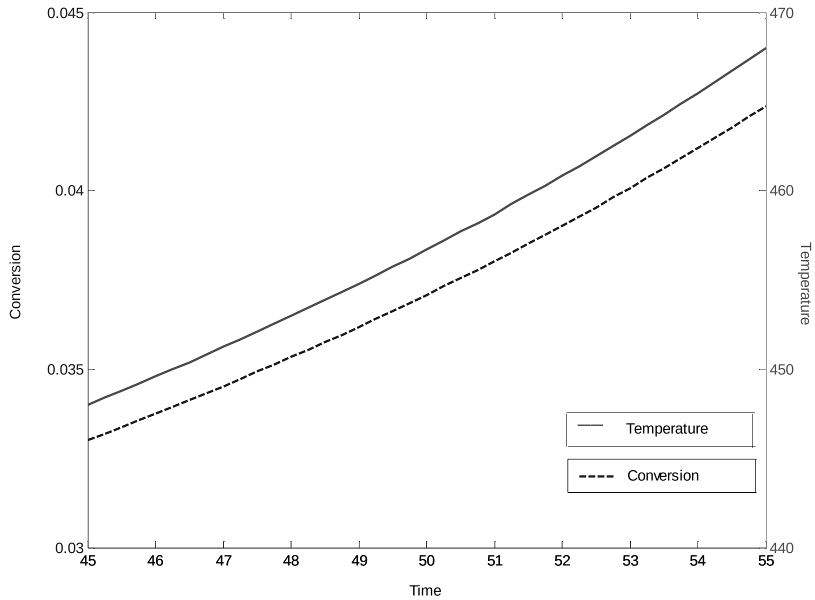


Figure S22.12b. *Adiabatic operation when the cooling is turned off.*

C.- BATCH OPERATION WITH HEAT EXCHANGE

Return of the cooling occurs at 55 min. The values at the end of the period of adiabatic operation are:

$t = 55 \quad T = 468 \text{ K} \quad X = 0.0423$

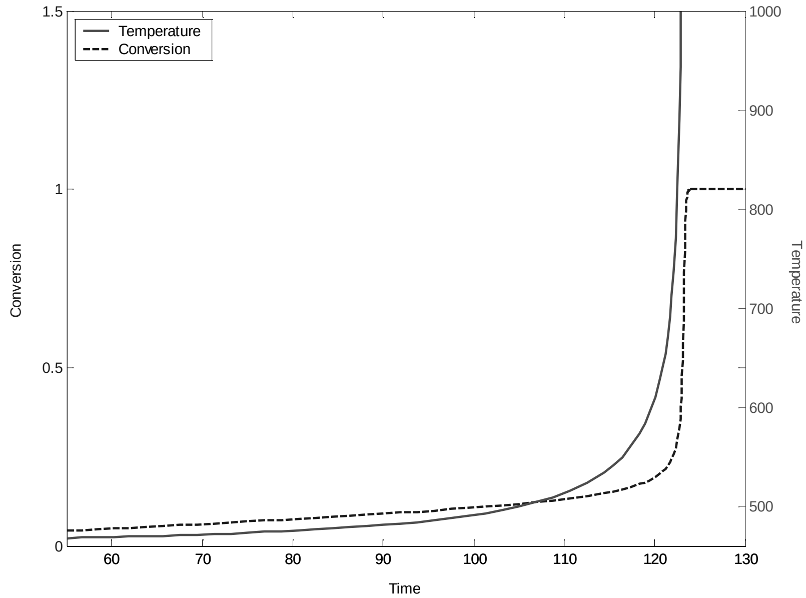


Figure S22.12c. *Batch operation with Heat Exchange; temperature runaway.*

As shown in Fig. S22.12c, the temperature runaway is finally unavoidable under new conditions:

. Feed composition = 9.044 kmol of ONCB, 33.0 kmol of NH_3, and 103.7 kmol of H_20

. Shut off cooling to the reactor at 45 minutes and resume cooling reactor at 55 minutes.

MATLAB simulation:

1.- Let's define the differential equation system in a file called reactor.

```
function dx_dt=reactor(t,x)

dx_dt(1,1)=((17e-5*exp(11273/1.987*(1/461-
1/x(2))))*1.767*(1-x(1))*(3.64-2*x(1)));

dx_dt(2,1)=((-(17e-5*exp(11273/1.987*(1/461-1/x(2))))*
122*(1-x(1))*(3.64-2*x(1))*5.119*(-5.9e5)  -
35.85*(x(2)-298))/2504 );
```

where `dx_dt(2,1)`the must be equal to 0 for the isothermal operation

2.- By using the command "ode45", system above can be solved

```
[times_row,x]=ode45('reactor',[to, tf],[X0,T0]);
plot(times_row,x(:,1),times_row,x(:,2));
```

where t_o, t_f, X_0 and T_0 must be specified for each interval.

22.13

T_r = Reactor temperature profile
T_{jsp} = Jacket set-point temperature profile (manipulated variable)

a) PID controller:

K_c = 26.5381
τ_I = 2.8658
τ_D = 0.4284

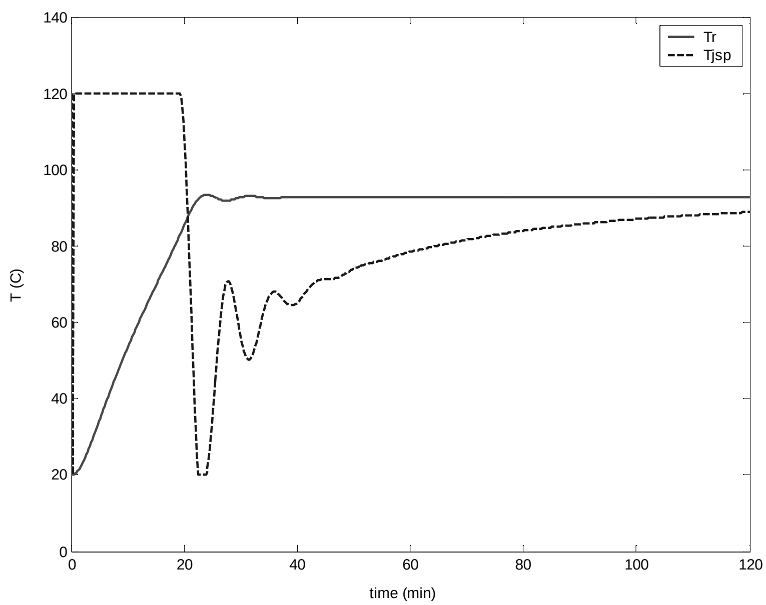


Figure S22.13a. *Numerical simulation for PID controller.*

b) Batch unit

K_c = 10.7574
τ_I = 53.4882

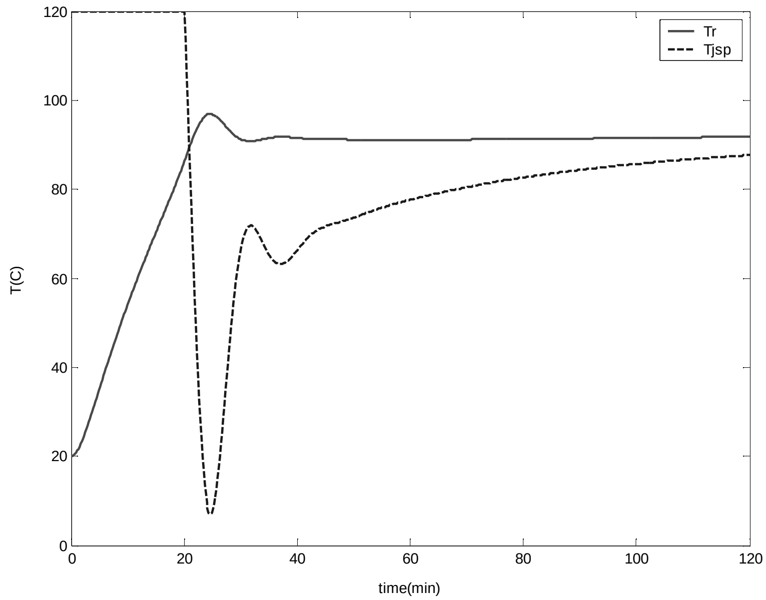


Figure S22.13b. *Numerical simulation for batch unit.*

c) Batch unit with preload

K_c = 10.7574
τ_I = 53.4882

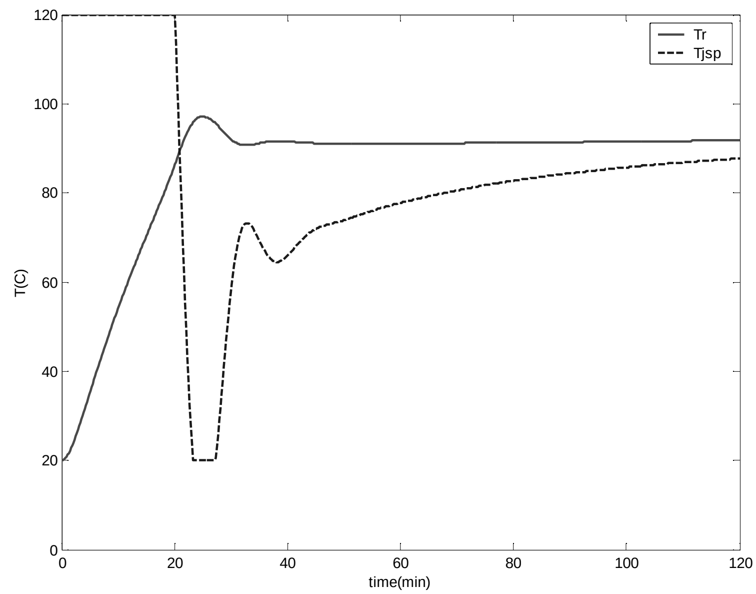


Figure S22.13c. *Numerical simulation for batch unit with preload.*

d) Dual mode controller

1.- Full heating is applied until the reactor temperature is within 5% of its set point temperature.
2.- Full cooling is then applied for 2.8 min
3.- The jacket temperature set point T_{jsp} of controller is then set to the preload temperature (46 °C) for 2.4 min.

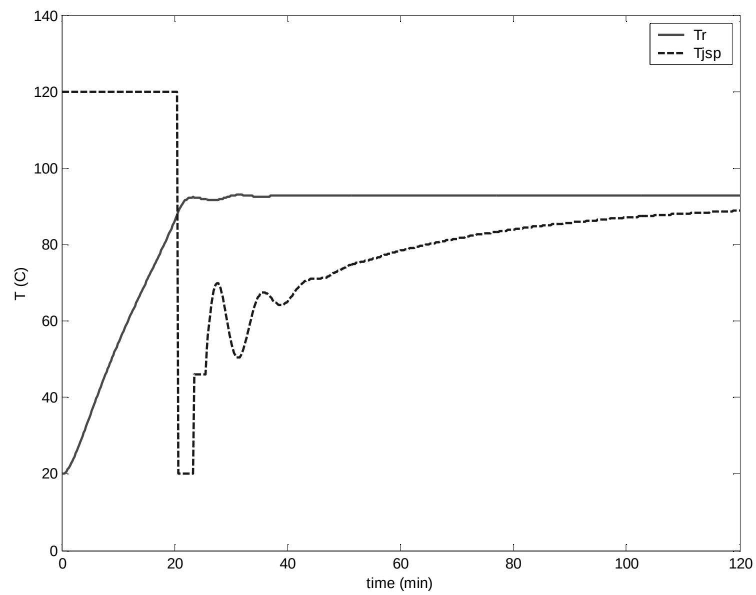


Figure S22.13d. *Numerical simulation for dual-mode controller.*

MATLAB simulation:

1.- Define a file called brxn:

```
function dy=brxn(t,y)
%
% Batch reactor example
%  Cott & Machietto (1989); "Temperature control
%  of exothermic batch reactors using generic model
%  control", I&EC Research, 28, 1177
%

% Parameters
 cpa=18.0; cpb=40.0; cpc=52.0; cpd=80.0;
 cp=0.45; cpj=0.45;
 dh1=-10000.0; dh2=6000.0;
 uxa=9.76*6.24;
 rhoj=1000.0;
 k11=20.9057; k12=10000;
 k21=38.9057; k22=17000;
 vj=0.6921;
 tauj=3.0;
 wr=1560.0;
```

```
dy=zeros(7,1);
ma=y(1); mb=y(2); mc=y(3); md=y(4); tr=y(5); tj=y(6);
tjsp=y(7);

k1=exp(k11-k12/(tr+273.15));
k2=exp(k21-k22/(tr+273.15));
r1=k1*ma*mb;
r2=k2*ma*mc;
qr=-dh1*r1-dh2*r2;
mr=ma+mb+mc+md;
cpr=(cpa*ma+cpb*mb+cpc*mc+cpd*md)/mr;
qj=uxa*(tj-tr);

dy(1)=-r1-r2;
dy(2)=-r1;
dy(3)=r1-r2;
dy(4)=r2;
dy(5)=(qr+qj)/(mr*cpr);
dy(6)=(tjsp-tj)/tauj-qj/(vj*rhoj*cpj);
dy(7)=0;
```

Note: The error between the reactor temperature and its set-point (e=cvsp-cv) is computed at each sampling time. That is, control actions are computed in the discrete-time. For the integral action, error is simply summated (se = se+e). Controller output is estimated by mv=Kc*e+Kc/taui*se*st, where Kc = proportional gain, taui=integral time, e=error, se=summation of error and st=sampling time

2.- PID controller simulation

```
clear
clf
%
%  batch reactor control system
%  PID controller (velocity form)
%

% process initial values
ma=12.0; mb=12.0; mc=0; md=0; tr=20.0; tj=20.0;
tjsp=20.0;

y0=[ma,mb,mc,md,tr,tj,tjsp];

% controller initial values
kc=26.5381; taui=2.8658; taud=0.4284;
en=0; enn=0;
cvsp=92.83; mv=20;

% simulation
st=0.2;
t0=0; tfinal=120;
ntf=round(tfinal/st)+1;
cvt=zeros(1,ntf); mvt=zeros(1,ntf);

for it=1:ntf
[tt,y]=ode45('brxn',[(it-1)*st it*st],y0);
 y0=y(length(y(:,1)),:);

 cv=y0(5);
```

```
% PID control calculation

e=cvsp-cv;
mv=mv+kc*(e*st/taui+(e-en)+taud*(e-2*en+enn)/st);
if mv>120, mv=120; elseif mv<20, mv=20; end
enn=en; en=e;

y0(7)=mv;

cvt(it)=cv; mvt(it)=mv;
end

t=(1:it)*st;
plot(t,cvt,'-r',t,mvt,'--g')
```

3.- Batch unit simulation

```
% controller
kc=10.7574; taui=53.4882;
mh=120; ml=20; mq=46;

mv=20;
cvsp=92.83;

% simulation
st=0.2;
z=ml; al=exp(-st/taui);
t0=0; tfinal=120;
ntf=round(tfinal/st)+1;

for it=1:ntf
[tt,y]=ode45('brxn',[(it-1)*st,it*st],y0);
y0=y(length(y(:,1)),:);

cv=y0(5);

e=cvsp-cv;
m=kc*e+z;

if m>mh, m=mh;
end
f=m
z=al*z+(1-al)*f; [f z m]

y0(7)=m;

cvt(it)=cv;
mvt(it)=m;
end

t=(1:it)*st;
plot(t,cvt,'-r',t,mvt,'-g');
```

4.- Batch unit with preload simulation

```
% controller
kc=10.7574; taui=53.4882;
```

```
 mh=120; ml=20; mq=46;
mv=20;
 cvsp=92.83;

  % simulation
  st=0.2;
  z=ml; al=exp(-st/taui);
  t0=0; tfinal=120;
  ntf=round(tfinal/st)+1;

  for it=1:ntf
  [tt,y]=ode45('brxn',[(it-1)*st,it*st],y0);
  y0=y(length(y(:,1)),:);
  cv=y0(5);
  e=cvsp-cv;
  m=kc*e+z;

  if m>mh, m=mh; else if m<ml, m=ml
  end
  end
  f=m
  z=al*z+(1-al)*f; [f z m]

  y0(7)=m;

  cvt(it)=cv;
  mvt(it)=m;
  end

  t=(1:it)*st;
  plot(t,cvt,'-r',t,mvt,'-g');
```

5.- Dual-mode simulation

```
clear
clf
%
%  batch reactor control system
%  dual-mode controller
%

% initial values
 ma=12.0; mb=12.0; mc=0; md=0; tr=20.0; tj=20.0;
 tjsp=20.0;

 y0=[ma,mb,mc,md,tr,tj,tjsp];

% controller initial values
 kc=26.5381; taui=2.8658; taud=0.4284;
en=0; enn=0;
cvsp=92.83;
td1=2.8; td2=2.4; pl=46; Em=0.95;
mv=20;
is=0;

% simulation
st=0.2;
t0=0; tfinal=120;
ntf=round(tfinal/st)+1;
cvt=zeros(1,ntf); mvt=zeros(1,ntf);

for it=1:ntf
```

```
[tt,y]=ode45('brxn',[(it-1)*st it*st],y0);
y0=y(length(y(:,1)),:);

cv=y0(5);

if is==0    %   heat up stage
 if cv<Em*cvsp
  mv=120;
 else
  is=1;
 tcool=it*st;
end
end

if is==1    %   cooling stage
 if it*st<tcool+td1
  mv=20;
 else
  is=2;
  tpre=it*st;
 end
end

if is==2   %   preload stage
 if it*st<tpre+td2
  e=cvsp-cv;
  mv=pl;
 else
  is=3;
 end
  enn=en; en=e;
 end

if is==3   %   control stage
  e=cvsp-cv;
 mv=mv+kc*(e*st/taui+(e-en)+taud*(e-
2*en+enn)/st);
  if mv>120, mv=120; elseif mv<20, mv=20; end
  enn=en; en=e;
end

 y0(7)=mv;

cvt(it)=cv;
mvt(it)=mv;
end
t=(1:it)*st;
plot(t,cvt,'-r',t,mvt,'-g')
```