\[ A \rightarrow B + C \quad \text{(irreversible)} \]

adiabatic PFR packed with catalyst

pure A enters reactor at a volumetric flowrate of \(20 \text{L/s} \)

\( P = 10 \text{ atm} \quad T = 450 \text{K} \)

\[ \begin{align*}
A & \rightarrow \\
& \quad \text{at} 450 \text{K} \\
& \quad \text{at} 10 \text{ atm}
\end{align*} \]

Plot conversion and \( T \) down reactor until an 80% conversion is reached

assume \( \Delta P = 0 \) (neglect pressure drop)

\[ \begin{align*}
C_p A &= 40 \text{ J/mol K} \\
C_p B &= 25 \text{ J/mol K} \\
C_p C &= 15 \text{ J/mol K}
\end{align*} \]

\[ \begin{align*}
H_A &= -70 \text{ kJ/mol} \\
H_B &= -50 \text{ kJ/mol} \\
H_C &= -210 \text{ kJ/mol}
\end{align*} \]

\[ \begin{align*}
H_i \text{ref} &= 278 \text{K} \\
K &= 0.33 \exp \left( \frac{E}{RT} \right)
\end{align*} \]

\[ \begin{align*}
E &= 31.4 \text{ kJ/mol}
\end{align*} \]

Mole balance:

\[ \frac{dF_A}{dw} = r_A \quad \frac{dF_B}{dw} = r_B \quad \frac{dF_C}{dw} = r_C \]

Rate Law:

\[ r_A = k \cdot C_A \]

Stoichiometry:

\[ \begin{align*}
C_A &= C_{\text{to}} \frac{F_A}{F_T} \frac{T_o}{T} \\
C_B &= C_{\text{to}} \frac{F_B}{F_T} \frac{T_o}{T} \\
C_C &= C_{\text{to}} \frac{F_C}{F_T} \frac{T_o}{T}
\end{align*} \]

Energy balance:

\[ \begin{align*}
\frac{dU}{dw} &= \frac{U_A(\text{T}_A - T) + (-r_A)(-\Delta H_A)}{F_A C_p A + F_B C_p B + F_C C_p C} \\
\text{adiabatic} \quad U(\text{T}_A - T) &= 0
\end{align*} \]
\[\frac{dT}{dw} = \frac{(-E_r)(-\Delta H_{rxn})}{F_{c,\text{in}} + T_0C_p\rho + F_cC_p}\]

\[\Delta H_{rxn} = \Delta H_{r,\text{in}}(T_0) + \int_{T_0}^{T} C_p dT = \Delta H_{r,\text{ex}}(T_0) \text{ because } \Delta C_p = 0\]

\[\Delta H_{r,\text{ex}}(T_0) = \frac{b}{a} H_{g,\text{in}}(T_0) + \frac{C}{a} H_{g,\text{in}}(T_0) - H_{s,\text{in}}(T_0)\]

See code and plots.

a) Plot conversion, T, and molar flow rates of A, B, C as a function of molar weight.
   
   for \(\Delta P = 0\) by setting \(\alpha = 0\)
   
   \(Q = 0\) by \(\frac{u_a}{\varepsilon} = 0\)

8-7/

Add Ergun equation to set of ode's:

\[\frac{dp}{dw} = -\frac{\alpha}{2} \left(\frac{T}{T_0}\right) \frac{P_0^2}{p} \left(\frac{E_r}{F_r}\right)\]

a) Plot T, conversion, and pressure along reactor

b) Vary \(\alpha\) and \(P_0\) to learn ranges of values in which they dramatically affect the conversion.

- Try 3 or 4 of each and watch plot of X vs. W.
  Describe what you see.
Add heat transfer effects to heat balance.

\[ \frac{U_a \Delta T}{P_0} = 0.8 \frac{J}{s \text{kgcat} K} \]  

(\text{NOTE: } \frac{U_a}{P_0} \text{ is the constant you use to get } \Delta T \text{ per kg cat, so you use 0.8 as your constant, no need to convert units})

For parts a, b, e, set \( \Delta P = 0 \) by setting \( d = 0 \).

a) What are the profiles if \( \frac{U_a}{P_0} \) were increased by a factor of 25?

- Show plots of conversion vs. \( W \) at both values of \( \frac{U_a}{P_0} \)

b) Make an estimate of the minimum entering \( T \) at which the reaction will ignite.
clear
global E deltaHref cto cpa cpb cpc To Ua alpha Po Fto

%Physical constants
alpha = 0.0075; % kg cat.
E = 31400; % J/mol

%Given constants
vo = 20; % L/s
Po = 10; % atm
To = 450; % K

cpa = 40; % J/mol K
cpb = 25; % J/mol K
cpc = 15; % J/mol K
Ha = -70000; % J/mol
Hb = -50000; % J/mol
Hc = -40000; % J/mol

% Calculated constants
cao = Po /(0.0821*To); % mol/L from ideal gas law
cto = cao; % pure A enters reactor
Fao = cao*vo; % mol/sec
Fto = Fao; % pure A enters reactor
deltaHref = Hb + Hc - Ha;
Ua = 0;

% set initial conditions
Fo(1) = Fao; % 1 = a
Fo(2) = 0; % 2 = b and no b in feed
Fo(3) = 0; % 3 = c and no c in feed
Fo(4) = To; % 4 = Temperature
% Fo(5) = Po; % 5 = Pressure

Wfin = 48; % Kg catalyst
Wspan = [0 Wfin];

% call ode solver to get F and T as a function of cat. weight
[W,F]=ode45('odeHW6', Wspan, Fo);

Fa = F(:,1);
Fb = F(:,2);
Fc = F(:,3);
T = F(:,4);
% P = F(:,5);

X = (Fao-Fa)/Fao;

plot(W,T);
xlabel('Cat. Weight (Kg)');
ylabel('Temperature (K)');
title('Problem 8.6')
function dF_aw = odeHW6(W,F)

global E deltaHref cto cpa cpb cpc To Ua alpha Po Fto

%calculate reaction parameters

k = 0.133*(exp((E/8.314)*((To^-1)-(F(4)^-1))));

deltaH = deltaHref;

Ft = F(1) + F(2) + F(3);

ra = -k*cto*F(1)*(Ft^-1)*To*F(4)^-1;
hra = -k*cto*F(1)*(Ft^-1)*To*(F(4)^-1)*F(5)*(Po^-1);

df_dw(1) = ra;
df_dw(2) = -ra;
df_dw(3) = -ra;

df_dw(4) = (Ua*(273-F(4)) + ra*deltaH)/(F(1)*cpa + F(2)*cpb + F(3)*cpc);

df_dw(5) = -(alpha/2)*Ft*(Fto^-1)*Po*Po*(F(5)^-1);

df_dw = df_dw';
Problem 8.6

Molar Flow Rates (mol/s)

Conversion

Temperature (K)
Varying $P_0$ does not affect conversion for this cat. weight.

$P_0$ will be important if your conversion is severely limited by pressure drop.
Problem 8.8 $U_a = 0.8$

- Flowrate (mol/s)
- Conversion
- Temperature (K)

Cat. Weight (Kg) vs. Flowrate (mol/s)
Cat. Weight (Kg) vs. Conversion
Cat. Weight (Kg) vs. Temperature (K)
Problem 8.8 \( U_a = 0.8 \times 25 \)

- **Flowrate (mol/s)**
  - 0 to 6
  - 0 to 50

- **Conversion**
  - 0 to 0.06
  - 0 to 50

- **Temperature (K)**
  - 460 to 320
  - 0 to 50

b) Minimum entering \( T_0 < 300 \text{ K} \)
f) Including pressure drop will change the heat balance in that it alters the volumetric flowrate. The gases will be cooled to a lower T for slow flowrates. As P decreases, \( \dot{V}_0 \) increases and cooling is not as efficient.
clear
global E deltaHref cto cpa cpb cpc To Ua alpha Po Fto

%Physical constants

for i = 1:5;
alphas = [.002 .005 .0075 .01 .02]; %Kg cat.
alpha = alphas(i);
%alpha = .0018;

E = 31400; %J/mol

%Given constants

vo = 20; %L/s
Po = 10; %atm
To = 450; %K

cpa = 40; %J/molK
cpb = 25; %J/molK
cpc = 15; %J/molK

Ha = -70000; %J/mol
Hb = -50000; %J/mol
Hc = -40000; %J/mol

%Calculated constants

cao = Po/(.0821*To); %mol/L from ideal gas law
cto = cao; %pure A enters reactor
Fao = cao*vo; %mol/sec
Fto = Fao; %pure A enters reactor
deltaHref = Hb + Hc - Ha;
Ua = 0;

%set initial conditions

Fo(1) = Fao; %1 = a
Fo(2) = 0; %2 = b and no b in feed
Fo(3) = 0; %3 = c and no c in feed
Fo(4) = To; %4 = Temperature
Fo(5) = Po; %5 = Pressure

Wfin = 30; %Kg catalyst
Wspan = [0 Wfin];

%call ode solver to get F and T as a function of cat. weight

[W,F]=ode45('odeHW6', Wspan, Fo);

Fa = F(:,1);
Fb = F(:,2);
Fc = F(:,3);
T = F(:,4);
P = F(:,5);

X = (Fao-Fa)/Fao;
Xalpha(:,i) = X;
end

Xalpha1 = Xalpha(:,1);
Xalpha2 = Xalpha(:,2);
Xalpha3 = Xalpha(:,3);
Xalpha4 = Xalpha(:,4);
Xalpha5 = Xalpha(:,5);

subplot(2,2,1), plot(W,P);
xlabel('Cat. Weight (Kg)');
ylabel('Pressure (atm)');
title('Problem 8.6');

subplot(2,2,2), plot(W,Walpha1,'b',W,Walpha2,'k',W,Walpha3,'r',W,Walpha4,'.b',W,Walpha5,'.k');
xlabel('Cat. Weight (Kg)');
ylabel('Conversion');
title('Problem 8.6');

subplot(2,2,3), plot(W,T);
xlabel('Cat. Weight (Kg)');
ylabel('Temperature (K)');
title('Problem 8.6');