Reactor Design I: Tutorial 2. Reactor Systems

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Question 1

Develop the stoichiometric table for case of a single reaction in which M reactants with varying stoichiometric coefficients react to product N products (also with varying stoichiometric ratios). The reaction may therefore be represented as follows:

$$r_1R_1 + r_2R_2 + ... + r_{M-1}R_{M-1} + r_MR_M \rightarrow p_1P_1 + p_2P_2 + ... + p_{N-1}P_{N-1} + p_NP_N$$

You may assume that the reaction is elementary.

Determine the mole fraction of each reactant as a function of conversion, if conversion is defined based on the amount of the first reactant (R_1) and if:

a) the reactor operates in the liquid phase (CSTR and PFR)
b) the reactor operates in the gas phase at less than 15 bar (CSTR and PFR)

Question 2

Consider the following reaction: $A + 2B \rightarrow C$ which has a reaction rate constant k = 0.23 and the reaction is elementary.

The reactor is fed with 50mol/s of A and 150 mol/s of B. All components remain in the liquid phase, and it may be assumed that the reaction mixture density is approximately that of water. The molar mass of A is 0.025kg.mol^{-1} whereas C is 0.060kg.mol^{-1}.

a) If a tank of volume 5.4m^3 containing a high speed mixer is available, what conversion is possible in the reactor?
b) If 3 tanks, each having a volume of 5.4m^3 containing a high speed mixers are available, what is the maximum possible conversion?

Question 3

Consider the following reaction: $2A + B \rightarrow 2C$ which has a reaction rate constant k = 1x10^{-7} , and it is known that the reaction is elementary. The reaction is to occur in a tubular packed (with catalyst) bed reactor.

The molar masses of A and B are 0.035kg/mol and 0.015kg/mol respectively. Density of the catalyst is 2500kg.m^{-3}, particle diameter is half a centimeter, diameter of a tube is 5cm, bed porosity is 0.55, reaction temperature 112^{0}C, rate constant is 1x10^{-7}, gas viscosity is 3x10^{-5}Pa.s.
Reactant feed: [F_A,F_B,F_C] = [100 50 0]. The feed flow to the reactor is at a pressure of 12atm.

Develop the conversion and pressure profiles over a 20kg catalyst tube.

Solutions

Question 1

Let's define conversion based on the very first species:

$$X = \frac{F_{R1,0} - F_{R1}}{F_{R1,0}}$$

For example, if we have the reaction:

$$A + 2B \rightarrow 3C$$

…then ν_A, ν_B, ν_C will be -1, -2 and 3 respectively (noting the negative for reactants).

If F_{A0} is the molar entry flowrate of component A then the molar flowrate after conversion X will be:

$$F_A = F_{A0} - F_{A0}X$$

Similarly, if F_{B0} is the molar entry flowrate of component B then the molar flowrate after conversion X will be:

$$F_B = F_{B0} - 2F_{A0}X$$

We may also define the inlet flow ratio as follows: $\Theta_i = F_{i0}/ F_{A0}$

And so get

$$F_B = F_{A0}\Theta_i - 2F_{A0}X$$

Let's also define the ratio of stoichiometric coefficients $\gamma_i = \nu_i/\nu_A$. We get:

$$F_B = F_{A0}\Theta_B - \gamma_B F_{A0}X = F_{A0}(\Theta_B - \gamma_B X)$$

More generally:

$$F_i = F_{A0}(\Theta_i - \gamma_i X)$$

Let's generalize our reaction from the R and P notation to the following form:
If we define ν_i to be the stoichiometric coefficient of the i-th component, then we can rewrite the reaction in the following way:

$$\sum_i \nu_i K_i = 0$$

Let's draw up the standard stoichiometric table:

Species	Initial	Remaining	Mole fraction
K_1	$F_{K1,0}$	$F_{K1,0}$ (1-X)	
K_2	$F_{K2,0}$	$F_{K1,0}$ (Θ_2-γ_2X)	
…	…	…	
K_{M+N-1}	$F_{KM+N-1,0}$	$F_{K1,0}$ (Θ_{M+N-1}-γ_{M+N-1}X)	
K_{M+N}	$F_{KM+N,0}$	$F_{K1,0}$ (Θ_{M+N}-γ_{M+N}X)	
Total	$\sum_{i=1}^{M+N} F_{Ki,0}$	$F_{K1,0}\sum_{i=1}^{M+N}(\Theta_i - \gamma_i X)$	

Mole fraction is then:

$$y_i = \frac{\Theta_i - \gamma_i X}{\sum_{i=1}^{M+N}(\Theta_i - \gamma_i X)}$$

To get concentration in the liquid phase, we need the volumetric flowrate. We start by getting the mass inlet flowrate as follows:

$$\dot{m}_{in} = \sum_i MM_i F_{Ki,0}$$

If the average density ρ is known, then we can get the volumetric flowrate: $v = \dot{m}_{in} / \rho$

In the liquid phase, the concentration will be:

$$c_i = \frac{F_{K1}(\Theta_i - \gamma_i X)}{v}$$

For gas phase reactions where the reaction rate is given as a function of partial pressures, the rate will be:

$$r' = kp_{R1}^{r1} p_{R2}^{r2} \ldots p_{RM}^{rM} = k\Pi_{i=1}^{M} p_{Ri}^{ri} = kp^{\sum_i ri} \Pi_{i=1}^{M} y_i = kp^{\sum_i ri} \Pi_{i=1}^{M} \frac{\Theta_i - \gamma_i X}{\sum_{i=1}^{M+N} (\Theta_i - \gamma_i X)}$$

The main point is that we now have: r = r(X)

In a similar way, we can get r = r(X) for the liquid phase.

a) Use the developments above and the design equation for the CSTR and PFR;
b) Use the developments above and the design equation for the CSTR and PFR

Question 2

The reaction is elementary, and therefore not first order.

We first need the molar mass of component B. Recognizing that mass must be conserved in the reaction, we have:

MMB = (MMC - MMA)/2

The mass entering the reactor must then be:

$$\dot{m}_{in} = \sum_i MM_i F_{Ki,0} = MM_A F_{A,0} + MM_B F_{B,0}$$

We are given that the density is approximately that of water (about 1000kg.m^{-3}) and so we can calculate:

$v = m_{in}/\rho$

The stoichiometric table gives us:

$F_A = F_{A0}(1-X)$;
$F_B = F_{B0} - 2F_{A0}X$;
$F_C = F_{A0}X$;

The mole fractions and concentrations then become:

FT = FA + FB + FC;
xA = FA./FT; xB = FB./FT; xC = FC./FT;
cA = FA/vin; cB = FB/vin; cC = FC/vin;

The reaction is elementary so we have:

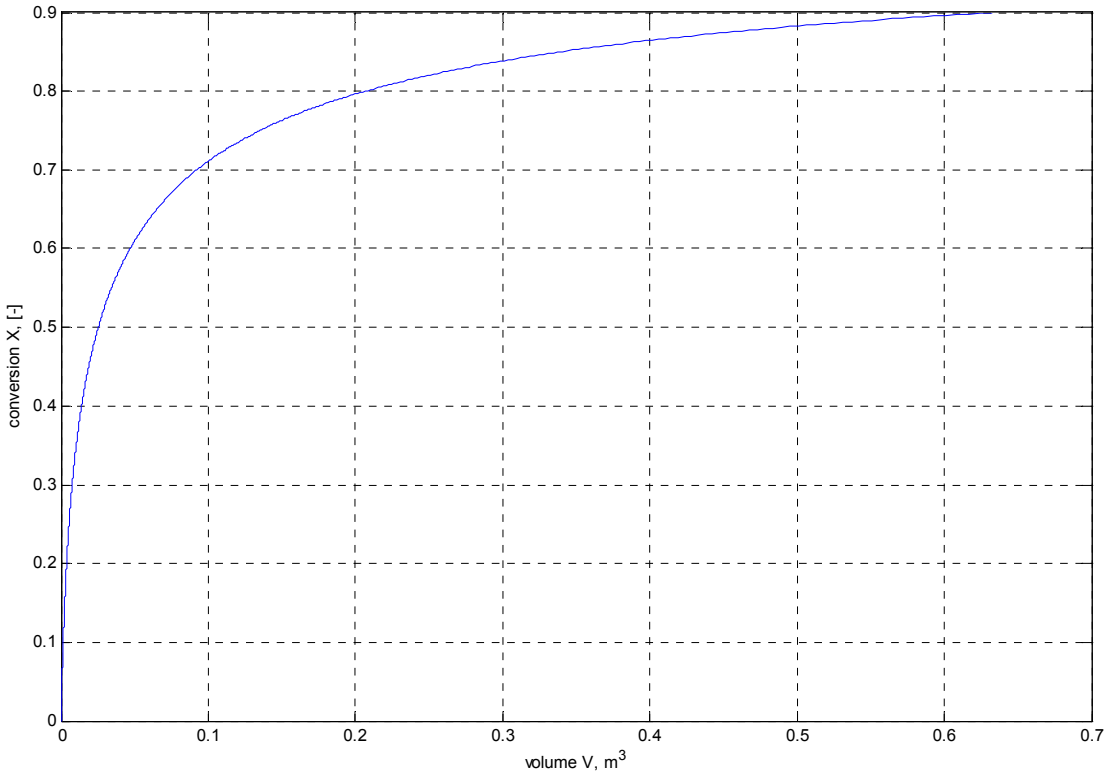
$r_A = kc_A c_B^2$

We can then use the CSTR design equation to get V = V(X).

The MatLab code looks like:

```
close all;clear all;clc

k = 0.23e-9;
MMA = 0.025; MMC = 0.06;
ro = 1e3; V = 5.4;
MMB = (MMC - MMA)/2 % Molar mass of component B

FA0 = 50; FB0 = 150; FC0 = 0;
min = FA0*MMA + FB0*MMB;
vin = min/ro; %m^3/s

X = linspace(0,0.9,1e3);

FA = FA0*(1-X);
FB = FB0 - 2*FA0*X;
FC = FA0*X;
% :-)
FT = FA + FB + FC;
xA = FA./FT; xB = FB./FT; xC = FC./FT;
cA = FA/vin; cB = FB/vin; cC = FC/vin;
rA = k*cA.*cB.^2;


V = FA0*X./rA;

plot(V,X)
xlabel('volume V, m^3')
ylabel('conversion X, [-]')
grid
```

And the solution looks like:



Question 3

The reaction is in the gas phase in a packed tube, so there might be appreciable pressure drop and hence loss of partial pressure and lowering of the reaction rate. We must therefore solve Ergun's equation simultaneously with the reaction. Our two differential equations are:

$$\frac{dp}{dW} = -\frac{G}{\rho_{gas} \cdot d_{Particle} \cdot \rho_{catalyst} \cdot A_c \cdot \phi^3} \cdot \left(150 \cdot \frac{(1-\phi) \cdot \mu}{d_{Particle}} + 1.75 \cdot G \right)$$

$$\frac{dX}{dW} = \frac{-r_A^{'}}{F_{A,0}}$$

(see class notes for derivation)

If we define conversion based on the inlet molar flowrate of component A, then the reaction stoichiometry yields:
$F_A = F_{A0}(1\text{-}X)$;
$F_B = F_{B0} - F_{A0}X/2$;
$F_C = F_{A0}X$;

The partial pressures may then be found as follows:
$y_i = F_i/\text{sum}(F_i)$
$p_i = y_i P$

The reaction rate is then

$$-r_A^{'} = k p_A^2 p_B$$

So much for the material balance (dX/dW). This development relies on us knowing the pressure P; we therefore still need the momentum balance dP/dW. Pretty much all the variables are nicely defined in the question or are easy to get, excepting the gas density. We calculate gas density as follows:
Average molar mass: $MMav = \text{sum}(MM_i y_i)$
Average density is then:

$$\rho = \frac{P.MM}{RT}$$

We can therefore solve this problem by writing some code. See next page.

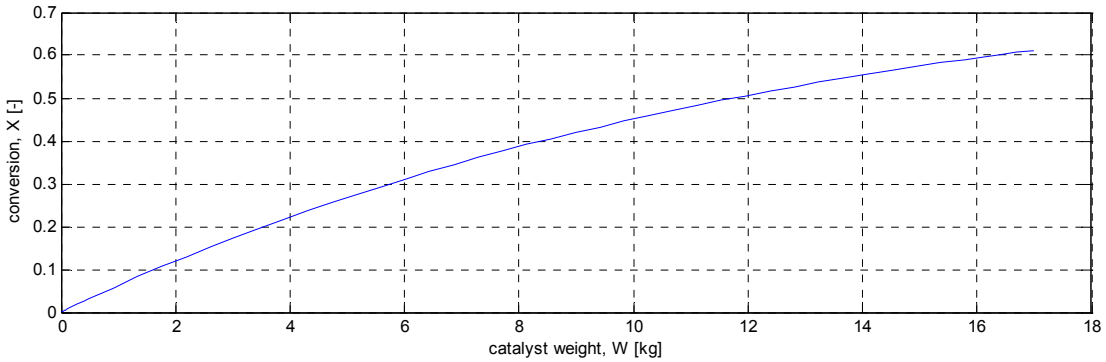
Differential Equations:

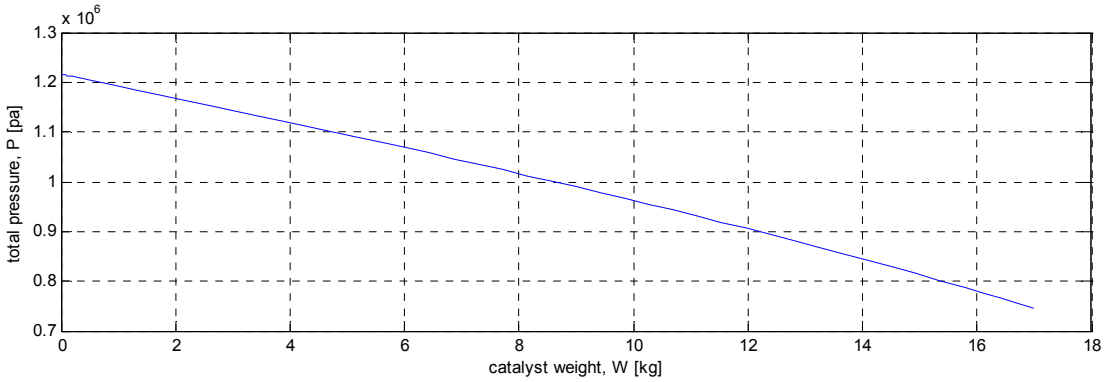
```
function dydW = dtut0203(W,y)

X = y(1);
P = y(2);

R = 8.314;
MMA = 35e-3; MMB = 15e-3; MMC = (2*MMA+MMB)/2;
MM = [MMA MMB MMC];
roc = 2500;
dp = .5e-2; % particle diameter
dr = 5e-2; % particle diameter
phi = 0.55;

T = 112 + 273.15; % reaction temperature
k = 1e-7;
mu = 3e-5;

p0 = 12*101325;
F0 = [100 50 0];

min = sum(F0.*MM);
Ac = pi/4*dr^2;
G = min/Ac;

dF0 = F0(1)*X;
F = F0 - [dF0 dF0/2 -dF0];
y = F/sum(F);
MMav = sum(MM.*y);
roav = P*MMav/R/T;

pi = p*y;
rA = k*pi(1)^2*pi(2);

dXdW = r/F0;
dPdW = -G/(roav*dp*roc*Ac*phi^3)*(150*(1-phi)*mu/dp+1.75*G);

dydW = [dXdW;dPdW];
```

Main program

```
close all;clear all;clc

Wspan = [0 20];
[W,y] = ode45(' dtut0203',Wspan,[0 12*101325]);

subplot(2,1,1),plot(W,y(:,1))
subplot(2,1,2),plot(W,y(:,2))
```

Result:


conversion, X [-]
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
2
4
6
8
10
12
14
16
18
catalyst weight, W [kg]


x 10^6
total pressure, P [pa]
1.3
1.2
1.1
1
0.9
0.8
0.7
0
2
4
6
8
10
12
14
16
18
catalyst weight, W [kg]