

UNIVERSITY OF ALBERTA
DEPARTMENT OF CHEMICAL ENGINEERING

Ch E 345 - Chemical Reactor Design
Seminar #1

January 20, 2017

1. Consider an ideal gas phase reaction



carried out in an isothermal batch reactor. The rate expression is

$$(-r_A) = k C_A C_B \quad k = 1 \times 10^{-5} \frac{\text{m}^3}{\text{mol} \cdot \text{s}}$$

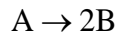
The reactor is charged with a mixture of 40 mol % A, 40 mol % B and 20 mol % inert. The temperature is constant at 100°C. The initial reactor pressure is 500 kPa. The reactor pressure is controlled during the course of the reaction such that the following relationship is valid

$$P_T = P_{T0} - a t \quad a = 1 \text{ Pa/s}$$

t is time in seconds and P_T and P_{T0} are the total pressure and initial total pressure in Pa.

Determine the time required to achieve 80% conversion of reactant A and the total reactor pressure at that time.

2. An irreversible gas phase reaction is conducted in an isothermal batch reactor. The overall reaction is:



The reactor is filled with a mixture of 70 mol % A and 30 mol % inert gas. The initial pressure is 90 kPa and the temperature is 400 K. The rate expression is 2nd order, that is $(-r_A) = k C_A^2$ and the rate constant has a value of $k = 0.75 \text{ m}^3/\text{mol} \cdot \text{h}$ at 400 K. Assume ideal gases.

- (a) Calculate the time required to achieve 60% conversion of A in a constant volume batch reactor.
- (b) Calculate the time required to achieve 60% conversion of A in a constant pressure batch reactor.

Solution to problem 1

This reaction is an ideal gas reaction carried out at variable pressure, with a change in moles on reaction. The volume may therefore change during the course of the reaction. The mole balance equation expressed in terms on moles is:

$$-\frac{1}{V} \frac{dN_A}{dt} = k C_A C_B = k \frac{N_A N_B}{V^2} \quad \text{Note: } N_A = N_B, \quad N_A = N_{A0}(1 - X_A)$$

Because the initial moles of A and B are equal, it follows that $N_A = N_B$ for all t . Writing the mole balance in terms of conversion for a batch reactor gives the following equation:

$$N_{A0} \frac{dX_A}{dt} = k \frac{N_{A0}^2}{V} (1 - X_A)^2 \quad \text{or} \quad \frac{dX_A}{dt} = k \frac{N_{A0}}{V} (1 - X_A)^2$$

The reactor volume can be related to the total pressure using the ideal gas law. Both pressure and number of moles change.

$$P_t V = N_t R_g T \quad \text{and} \quad P_{t0} V_0 = N_{t0} R_g T$$

Dividing by the conditions at $t = 0$ gives:

$$\frac{P_{t0} V_0}{P_t V} = \frac{N_{t0}}{N_t} \quad \text{or} \quad V = \frac{N_t}{N_{t0}} \frac{P_{t0} V_0}{P_t}$$

To determine N_t develop a mole balance table:

Compound	Moles Initial	Moles at t
A	N_{A0}	$N_{A0}(1 - X_A)$
B	N_{A0}	$N_{A0}(1 - X_A)$
C	0	$N_{A0}X_A$
I	$0.5N_{A0}$	$0.5N_{A0}$
Total	$2.5N_{A0}$	$2.5N_{A0} - N_{A0}X_A$

Therefore the mole ratio is:

$$\frac{N_t}{N_{t0}} = \frac{N_{A0}(2.5 - X_A)}{2.5N_{A0}} = 1 - 0.4X_A$$

Substituting for the pressure gives:

$$V = \frac{(1 - 0.4 X_A) P_{t0}}{P_{t0} - a t} V_0$$

By substitution into the batch reactor mole balance equation:

$$\frac{d X_A}{d t} = \frac{k N_{A0}}{V_0 P_{t0}} (P_{t0} - a t) \frac{(1 - X_A)^2}{(1 - 0.4 X_A)}$$

In integral form:

$$\int_0^{0.8} \frac{1 - 0.4 X_A}{(1 - X_A)^2} d X_A = \frac{k N_{A0}}{V_0 P_{t0}} \int_0^t (P_{t0} - a t) d t$$

Integrating gives:

$$\left[\frac{1}{1 - X_A} - 0.4 \left(\ln(1 - X_A) + \frac{1}{(1 - X)} \right) \right]_0^{0.8} = \left[\frac{k N_{A0}}{V_0 P_{t0}} \left(P_{t0} t - \frac{a}{2} t^2 \right) \right]_0^t$$

The left-hand side is equal to 3.04 and $N_{t0} = 2.5 N_{A0}$. Therefore we may write:

$$3.04 = \frac{k N_{t0}}{2.5 V_0 P_{t0}} \left(P_{t0} t - \frac{a}{2} t^2 \right)$$

From the ideal gas law:

$$\frac{N_{t0}}{V_0 P_{t0}} = \frac{1}{R_g T}$$

Therefore:

$$3.04 = \frac{k}{2.5 R_g T} \left(P_{t0} t - \frac{a}{2} t^2 \right)$$

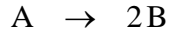
Substituting for the problem parameters gives:

$$2.36 \times 10^9 - 5 \times 10^5 t + \frac{1}{2} t^2 = 0$$

Solving this quadratic equation for t gives two solutions: $t = 4742s$ and $t = 1 \times 10^6 s$. The solution at 4742 s is achieved first and thus is the answer.

Solution to problem 2

The overall reaction is given by the stoichiometry:



with a feed of 70% A and 30% inerts. The reaction rate follows a second order expression:

$$(-r_A) = k C_A^2 \quad \text{where} \quad k = 0.75 \frac{\text{m}^3}{\text{mol} \cdot \text{h}}$$

This reaction occurs in the gas phase with an increase in the number of moles on reaction.

Part (a)

For the constant volume batch reactor the change in moles on reaction will not affect the concentration. Rather the pressure will increase as B is formed. The mole balance equation written in terms of the concentration for a constant volume batch reactor (CVBR) is:

$$-\frac{dC_A}{dt} = k C_A^2$$

Written in terms of the fractional conversion the mole balance is:

$$\frac{dX_A}{dt} = k C_{A0}(1 - X_A)^2$$

Writing the equation in integral form with the final limit of $X_A = 0.6$ gives:

$$\int_0^{0.6} \frac{dX_A}{(1 - X_A)^2} = k t C_{A0} = \frac{1}{1 - X_A} \Big|_0^{0.6}$$

Using the ideal gas law for C_{A0} gives:

$$C_{A0} = \frac{P_0 Y_{A0}}{R_g T} = \frac{(90,000)(0.7)}{(8.314)(400)} = 18.94 \frac{\text{mol}}{\text{m}^3}$$

Multiply by the rate constant to give a value of $k C_{A0} = 14.21 \text{ h}^{-1}$. Substituting this value into the integrated mole balance equation above gives:

$$14.21 t = \left(\frac{1}{0.4} - \frac{1}{1} \right)$$

Solution gives a value of $t = 0.11 \text{ h}$ or 380 s .

Part (b)

In a constant pressure batch reactor, the volume will increase as B is produced, because of the change in the number of moles with reaction. It is therefore preferable to work in terms of the number of moles rather than the concentration. The mole balance equation is thus written as:

$$-\frac{1}{V} \frac{dN_A}{dt} = k C_A^2 = k \left(\frac{N_A}{V} \right)^2$$

Simplification gives:

$$-\frac{dN_A}{dt} = \frac{1}{V} k N_A^2$$

Expressing in terms of the initial moles and the fractional conversion gives:

$$\frac{dX_A}{dt} = \frac{N_{A0}}{V} k (1 - X_A)^2$$

The relationship between the total number of moles N_t and the volume V at constant pressure and temperature is obtained from the ideal gas law:

$$V = V_0 \frac{N_t}{N_{t0}}$$

The subscript "0" denotes initial conditions. The volume can then be related to the conversion by expressing the total number of moles in terms of conversion. The mole balance table can be written in terms of the initial total moles present as:

Compound	Initial Moles	Final Moles
A	$0.7 N_{t0}$	$0.7 N_{t0}(1 - X_A)$
B	0	$0.7 N_{t0} (2 X_A)$
I	$0.3 N_{t0}$	$0.3 N_{t0}$
Total	N_{t0}	$N_{t0}(1 + 0.7 X_A)$

From part (a) we have $k C_{A0} = 14.21 \text{ h}^{-1}$. Substitution into the mole balance equation gives:

$$\frac{dX}{dt} = k C_{A0} \frac{(1-X_A)^2}{(1+0.7X_A)} = 14.21 \frac{(1-X_A)^2}{(1+0.7X_A)}$$

In integral form:

$$\int_0^{0.6} \frac{(1+0.7X)}{(1-X)^2} dX_A = 14.21 t$$

This equation can be integrated analytically:

$$\left[\frac{1}{1-X_A} + \frac{0.7}{1-X_A} + 0.7 \ln(1-X_A) \right]_0^{0.6} = 14.21 t$$

Substituting the limits gives:

$$t = \frac{1}{14.21} \left[1.7 \left(\frac{1}{1-0.6} - \frac{1}{1} \right) + 0.7 \ln \left(\frac{1-0.6}{1} \right) \right]$$

Solution gives $t = 0.13$ h or 483.5 s . Note that the reactor volume increase effectively reduces the reactant concentration; hence the rate of reaction is also reduced and it takes longer to reach the desired conversion, as compared to a constant volume batch reactor.