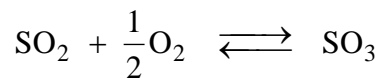


**UNIVERSITY OF ALBERTA
DEPARTMENT OF CHEMICAL ENGINEERING**

**Ch E 345 - Chemical Reactor Design 1
Seminar #6**

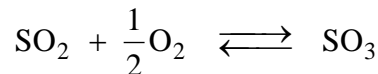
March 10, 2017

1. The gas from a sulphur burner consists of 8 mol % SO₂, 11 mol % O₂ and 81 mol % N₂. This gaseous mixture is passed to a catalytic reactor where SO₂ is oxidized to SO₃. The reactor exit temperature is 500°C and the pressure is 1 bar. The equilibrium constant at 500°C is 85 and fugacity coefficients are essentially equal to one. Calculate the reactor exit conversion if equilibrium is established. The reaction is:



Repeat the calculation for a total pressure of 2 bar.

2. Consider the oxidation of sulphur dioxide to sulphur trioxide, given by the reaction:

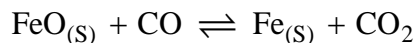


The equilibrium constant is 85 at 500°C. The enthalpy of reaction is -98.2 kJ/mol of SO₂ converted, and may be assumed constant. The heat capacities of the species may be assumed to have constant values of:

N₂ 28.8 J/mol O₂ 32.6 J/mol SO₂ 47.7 J/mol SO₃ 64.0 J/mol

A mixture of SO₂, O₂ and N₂ enter an adiabatic oxidation reactor. The mixture reacts and comes to equilibrium. Calculate the final temperature of the mixture if the initial temperature is 400°C. The initial composition of the mixture is 8 mol % SO₂, 11 mol % O₂ and 81 mol % N₂. The total pressure is 100 kPa (1 bar).

3. Ferrous oxide is reduced to iron in the reaction:



A mixture of 20 % CO and 80 % N₂ is passed over the FeO at a temperature of 1273 K and a pressure of 1 bar. If equilibrium is reached, compute the mass of Fe produced per m³ of gas admitted. The gas volume is referenced at a temperature of 1273 K and a pressure of 1 bar. At 1273 K the equilibrium constant has a value of 0.403. Assume ideal gases.

Solution to problem 1

The equilibrium constant at 500°C has a value of 85. The relationship between composition and the equilibrium constant K is:

$$K = \frac{K_y K_\phi}{K_{f_i^\circ}} P^{\sum v_i}$$

From the reaction stoichiometry the change in moles on reaction is:

$$\sum v_i = 1 - 1 - \frac{1}{2} = -\frac{1}{2}$$

Because the fugacity coefficients are equal to one, it follows that $K_\phi = 1$. Using a standard state of 1 bar gives:

$$K = K_y P^{-0.5} \quad \text{where } P \text{ is in bar}$$

The mole fractions at equilibrium must be expressed in terms of the number of moles present at equilibrium. Take a basis of 100 moles of original mixture and let X be the fractional conversion at equilibrium. That is,

$$X = \frac{N_{\text{SO}_2,0} - N_{\text{SO}_2}}{N_{\text{SO}_2,0}}$$

Construct a stoichiometric table on the 100 mole basis:

Compound	Moles Initial	Moles Final
SO ₂	8	8(1 - X)
SO ₃	0	8X
O ₂	11	11 - $\frac{8}{2}X$
N ₂	81	81
Total	100	100 - 4X

Substitute into the equation for K :

$$K = K_y P^{-0.5} = \frac{y_{\text{SO}_3}}{y_{\text{SO}_2} y_{\text{O}_2}^{0.5}} \times 1^{-0.5} = \frac{\left(\frac{8X}{100-4X}\right)}{\left(\frac{8(1-X)}{100-4X}\right)\left(\frac{11-4X}{100-4X}\right)^{0.5}} = 85$$

Simplify:

$$85 = \frac{X}{1-X} \left(\frac{100-4X}{11-4X} \right)^{0.5}$$

The above equation is solved numerically to get a value of $X = 0.9587$. Therefore at equilibrium 95.87% of the original SO_2 is converted to SO_3 .

At 2 bar pressure the equation becomes:

$$85 = 2^{-0.5} \frac{X}{1-X} \left(\frac{100-4X}{11-4X} \right)^{0.5}$$

Solving numerically gives a value of $X = 0.97$. Note that an increase in pressure gives an increase in conversion.

Solution to problem 2

The reactor is adiabatic so the energy released by the reaction heats up the process stream. Take a basis of 100 moles of mixture. First calculate ΔC_P for the reaction using the values supplied.

$$\Delta C_P = (C_P)_{\text{SO}_3} - \frac{1}{2}(C_P)_{\text{O}_2} - (C_P)_{\text{SO}_2} = 64.0 - \frac{1}{2}32.6 - 47.7 = 0$$

It is seen that $\Delta C_P = 0$ which means that the heat of reaction is constant (it does not change with temperature) and the heat capacity of the feed may be used to represent the mean heat capacity of the mixture. Let X be the fractional conversion of SO_2 , then the mole balance table is

Compound	Moles Initial	Moles Final
SO_2	8	$8(1 - X)$
SO_3	0	$8X$
O_2	11	$11 - 4X$
N_2	81	81
Total	100	$100 - 4X$

The heat released on reaction is the product of the enthalpy of reaction and the moles of SO_3 that react, or $8X(-\Delta H_R)$. The heat capacity of 100 moles of feed is

$$\bar{C}_P = 8 \times 47.7 + 11 \times 32.6 + 81 \times 28.8 = 3073 \text{ J}$$

The energy balance therefore gives:

$$(-\Delta H_R)8X = \int_{673}^T \bar{C}_P dT = 3073(T - 673)$$

Substitute for $-\Delta H_R$, X and simplify to give the adiabatic reaction line:

$$T = 255.6X + 673 \quad (1)$$

where T is in Kelvin. The relationship between composition and the equilibrium constant K is:

$$K = \frac{K_y K_\phi}{K_{f_i}^\circ} P^{\sum v_i}$$

From the reaction stoichiometry the change in moles on reaction is:

$$\sum v_i = 1 - 1 - \frac{1}{2} = -\frac{1}{2}$$

The fugacity coefficients are equal to one, therefore $K_\phi = 1$. With a standard state of 1 bar:

$$K = K_y P^{-0.5} \quad \text{where } P \text{ is in bar}$$

The mole fractions at equilibrium must be expressed in terms of the number of moles present at equilibrium. Take a basis of 100 moles of original mixture and let X be the fractional conversion at equilibrium. That is:

$$X = \frac{N_{\text{SO}_2,0} - N_{\text{SO}_2}}{N_{\text{SO}_2,0}}$$

Substitute into the equation for K :

$$K = K_y P^{-0.5} = \frac{y_{\text{SO}_3}}{y_{\text{SO}_2} y_{\text{O}_2}^{0.5}} \times 1^{-0.5} = \frac{\left(\frac{8X}{100-4X} \right)}{\left(\frac{8(1-X)}{100-4X} \right) \left(\frac{11-4X}{100-4X} \right)^{0.5}}$$

Simplify:

$$K = \frac{X}{1-X} \left(\frac{100-4X}{11-4X} \right)^{0.5} \quad (2)$$

The temperature dependence of K is given by:

$$\frac{d \ln K}{dT} = \frac{\Delta H_R^\circ}{R_g T^2}$$

As ΔH_R° is assumed constant, this equation can be integrated to give:

$$\ln \frac{K_2}{K_1} = \frac{(-\Delta H_R^\circ)}{R_g} \left[\frac{1}{T_2} - \frac{1}{T_1} \right]$$

or, by rearrangement:

$$\frac{1}{T_2} = \frac{1}{T_1} + \frac{R_g}{(-\Delta H_R^\circ)} \ln \left(\frac{K_2}{K_1} \right)$$

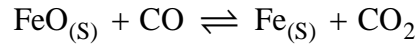
Substitute the known value of $K = 85$ at 500°C .

$$\frac{1}{T} = \frac{1}{773} + \frac{8.314}{98.2 \times 10^3} \ln \left(\frac{K}{85} \right) \quad (3)$$

Equations (1), (2), and (3) can be solved numerically to give $X = 0.798$ and $T_2 = 876.9 \text{ K}$.

Solution to problem 3

Ferrous oxide is reduced to iron in the reaction:



For an ideal gas we can write the equilibrium constant in terms of the gas phase mole fractions, recalling that the activity of the solid is equal to one.

$$K = \frac{Y_{\text{CO}_2}}{Y_{\text{CO}}} = 0.403$$

The mole fractions can be expressed in terms of the fractional conversion of CO at equilibrium:

$$\begin{aligned} Y_{\text{CO}} &= (Y_{\text{CO}})_0 (1 - X) \\ Y_{\text{CO}_2} &= (Y_{\text{CO}})_0 X \end{aligned}$$

Substitute into the expression for the equilibrium constant:

$$K = \frac{(Y_{\text{CO}})_0 X}{(Y_{\text{CO}})_0 (1 - X)} = 0.403$$

Solve for $X=0.287$. Thus, for each mole of CO admitted, 0.287 mole of $\text{Fe}_{(s)}$ is produced.

Therefore, for each mole of entering gas,

$$(0.287) (0.20) = 0.0574$$

mole of Fe is produced. For 1 m³ of gas, the number of moles is:

$$n = \frac{PV}{R_g T} = \frac{(101325)(1)}{(8.314)(1273)} = 9.57 \text{ mol}$$

Therefore 0.55 mole of Fe is produced per cubic metre of entering gas.