The University of Calgary
Department of Chemical & Petroleum Engineering

ENCH 501: Mathematical Methods in Chemical Engineering
Quiz #2

Time Allowed: 50 mins. **September 26, 2000**

Student's Name: ______________________

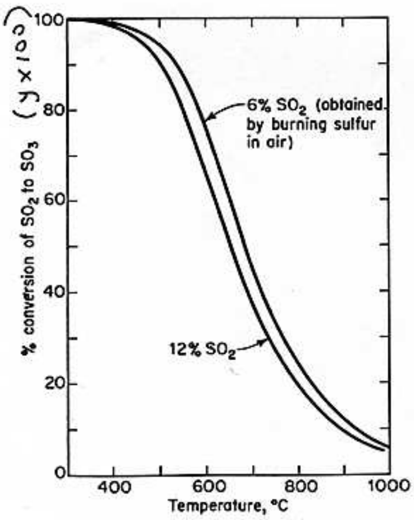
Sulphur trioxide *(SO_3)* involved in H_2SO_4 manufacture is obtained by oxidizing sulphur dioxide *(SO_2)* with air. The exothermic reactions from elemental sulphur and oxygen are:

(1) $S_{(g)} + O_{2_{(g)}} \rightarrow SO_{2_{(g)}}$; $\Delta H_r = -196.6\ kJ/mol$

(2) $SO_{2_{(g)}} + \frac{1}{2} O_{2_{(g)}} \Leftrightarrow SO_{3_{(g)}}$; $\Delta H_r = -97.9\ kJ/mol$

ΔH_r is heat of reaction.

The percent conversion of SO_2 to SO_3 depends on the concentration of SO_2 in the gases from reaction (1). Data from one such process is provided in the following plot:



Equilibrium-temperature relation for SO_2 conversion to SO_3. *(Monsanto Co.)*

The equilibrium constants for the process at different temperatures but a total pressure of 1 atm. Is given in the table below:

TABLE *Equilibrium Constants for Sulfur Dioxide Oxidation*

Temperature, °C	K_p	Temperature, °C	K_p
400	397	800	0.915
500	48.1	900	0.384
600	9.53	1000	0.1845
700	2.63	1100	0.0980

Source: Z. Elektrochem., **11**, 373 (1905).

~~From~~ For equation (2) above:

$$K_P = \frac{P_{SO_3}}{P_{SO_2} \times P_{O_2}^{\;1/2}}$$

and,

$$P_{SO_2} = \frac{2x_F\,(1-y)}{2 - x_F\,y}$$

$$P_{SO_3} = \frac{2x_F\,y}{2 - x_F\,y}$$

$$P_{O_2} = \frac{0.42 - x_F\,(2+y)}{2 - x_F\,y}$$

where x_F is the initial volume fraction of SO_2 in the feed gas into the $SO_2 - to - SO_3$ converter, and y is the equilibrium conversion (~~form~~ from the plot).

For a particular process, the exact concentration of SO_2 in the gases from the sulphur burner is not known but suspected to be between 8 and 10%. The temperature is measured as 600°C.

(a) Estimate the value and error for K_P. Compare with the value in the table.

(b) Estimate the heat released (and the error) for each mole of elemental sulphur consumed.

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(a) The concentration of SO_2 from reaction 1 is suspected to be between 8 and 10 %. Use 9 ± 1 %.

That is $x_F = 0.09 \pm 0.01$

from the plot $y = 71.4 \pm 1.5\%$ or 0.714 ± 0.015

Now use the expressions provided. See Lecture Notes.

(SO_2) $P_{SO_2} = \dfrac{2x_F - 2x_F y}{2 - x_F y}$ $x_F = 0.09(1 \pm 0.11)$

$y = 0.714(1 \pm 0.021)$

{Division / Multiplication, add relative errors $\Delta(x_F y)_r = 0.11 + 0.021$

$= 0.131$

$x_F y = (0.09)(0.714)(1 \pm 0.131)$

$= 0.064260 \pm 0.008418$

{Subtraction / Addition, add absolute errors

$2x_F - 2x_F y = 2(0.09 - 0.06426) \pm \{2(0.01) + 2(0.00842)\}$

$= 0.05148 \pm 0.036836$

$= 0.05148(1 \pm 0.71554)$

$2 - x_F y = (2 - 0.06426) \pm 0.008418$

$= 1.93574 \pm 0.008418$

$= 1.93574(1 \pm 0.004349)$

$P_{SO_2} = \dfrac{0.05148}{1.93574}(1 \pm \{0.71554 + 0.004349\})$

$= 0.026594(1 \pm 0.79889)$

(SO_3) $P_{SO_3} = \dfrac{2x_F y}{2 - x_F y}$

From above

$$P_{SO_3} = \frac{2(0.06426)}{1.93574}\left\{1 \pm \left[2(0.131) + 0.004349\right]\right\}$$

$$= 0.066393\left\{1 \pm 0.266349\right\}$$

(O_2) $$P_{O_2} = \frac{0.42 - x_F(2+y)}{2 - x_F y}$$

$$0.42 - 2x_F - x_F y = \left[0.42 - 2(0.09) - 0.06426\right] \pm \left[2(0.01) + 0.008418\right]$$

$$= 0.17574 \pm 0.028418$$

$$= 0.17574\,(1 \pm 0.161705)$$

$$P_{O_2} = \frac{0.17574}{1.93574}\left(1 \pm (0.161705 + 0.004349)\right)$$

$$= 0.090787\,(1 \pm 0.166054)$$

$$= 0.090787 \pm 0.015076$$

$$K_p\Big|_{600} = \frac{0.0664}{(0.0266)(0.0908)^{\frac{1}{2}}} = 8.29$$

Error

$$\Delta K_p = \frac{1}{P_{SO_2} P_{O_2}^{\frac{1}{2}}}\left(\pm \Delta P_{SO_3}\right) - \frac{P_{SO_3}}{(P_{SO_2})^2 (P_{O_2}^{\frac{1}{2}})}\left(\pm \Delta P_{SO_2}\right)$$

$$- \frac{1}{2}\frac{P_{SO_3}}{P_{SO_2} P_{O_2}^{3/2}}\left(\pm \Delta P_{O_2}\right)$$

Substitute values calculated above

$$\pm \Delta K_p = \frac{1}{(0.0266)(0.0908)^{\frac{1}{2}}} (0.246)(0.0664) \quad +$$

$$\frac{0.0664}{(0.0266)^2 (0.0908)^{\frac{1}{2}}} (0.799)(0.0266) \quad +$$

$$\frac{1}{2} \frac{(0.0664)}{(0.0266)(0.0908)^{3/2}} (0.166)(0.0908)$$

$$=$$

$\therefore \quad K_p = 8.29 \pm 9.51$ Large error range. (Low accuracy.)

From the table, $K_p = 9.53$ at $600°C$

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b The heat released per mole $S_{(g)}$

$$Q = 196.6 + 0.714(97.9)(1 \pm 0.021)$$

$$= 266.5 \pm 1.47 \text{ kJ}$$

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