The University of Calgary
Department of Chemical & Petroleum Engineering

ENCH 501: Mathematical Methods in Chemical Engineering
Quiz #2

Time Allowed: 30 mins. **September 25, 2001**

Problem #1

A reversible reaction A + B ⇌ 2C has the following rate expression for production of C:

$$r = k_1 C_A^{\frac{3}{2}} C_B^{\frac{1}{2}} - k_2 C_C^2$$

Given the following data:

$k_1 = 6.7\ (10^{-4}) \pm 0.5\ (10^{-4})$ litre/mol · min

$k_2 = 1.2\ (10^{-4}) \pm 0.2\ (10^{-4})$ litre/mol · min

$C_A = 3.5 \pm 0.3$ mols/litre

$C_B = 4.81 \pm 0.6$ mols/litre

$C_C = 2.6 \pm 0.1$ mols/litre

Estimate the rate at which compound C is being produced and the error in the rate.

Solution Quiz #2 ENCH 501 Sept 25, 2001

$$r = k_1 C_A^{3/2} C_B^{1/2} - k_2 C_C^2$$

Observed rate

$$r = (6.7)(10^{-4})(3.5)^{3/2}(4.81)^{1/2} - 1.2(10^{-4})(2.6)^2$$

$$= 0.009622 - 0.000811 = 0.00881 \ \frac{\text{moles}}{\text{litre} \cdot \text{min}}$$

Error. $r = f(k_1, k_2, C_A, C_B, C_C)$

$$dr = \frac{\partial r}{\partial k_1}\Delta k_1 + \frac{\partial r}{\partial k_2}\Delta k_2 + \frac{\partial r}{\partial C_A}\Delta C_A + \frac{\partial r}{\partial C_B}\Delta C_B + \frac{\partial r}{\partial C_C}\Delta C_C$$

$$= \left(C_A^{3/2} C_B^{1/2}\right)\Delta k_1 + \left(-C_C^2\right)\Delta k_2 + \left(k_1 C_B^{1/2} \cdot \frac{3}{2} C_A^{1/2}\right)\Delta C_A +$$

$$\left(k_1 C_A^{3/2} \cdot \frac{1}{2} C_B^{-1/2}\right)\Delta C_B + \left(-k_2 \cdot 2 C_C\right)\Delta C_C$$

Now evaluate each of the terms. (Remember each Δk_1, Δk_2 ... and both + and -ve. To maximize error, add the absolute for each term.)

$$dr = (14.36)(0.5)(10^{-4}) + (6.74)(0.2)(10^{-4}) +$$

$$\left\{6.7(10^{-4})(2.193)(1.87)(1.5)\right\} 0.3 + (6.7)(10^{-4})(3.5)^{3/2}(0.5)$$

$$(4.81)^{-0.5}(0.6) + (1.2)(10^{-4})(2)(2.6)(0.1)$$

$$= 0.002753$$

$$\therefore \quad r = 0.00881 \pm 0.002753 \ \text{moles/litre} \cdot \text{min}$$

The error is 31.2% !