Kinetics and Reactor Design HW9

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Assigned: April 4, 2023
Due: April 18, 2023

1 Problem Statement

1.1 P11-2_A

P11-2_A For elementary reaction

$$A \rightleftarrows B$$

the equilibrium conversion is 0.8 at 127°C and 0.5 at 227°C. What is the heat of reaction?

Figure 1

1.2 Question 2

Derive an expression for the equilibrium constant $K_C(T)$ solely as a function of $K_C(T_1)$, $\Delta\varepsilon\lambda\tau\alpha C_P$, $\Delta H^o_{Rx}(T_R)$, T, T_1, T_R, and the gas constant R for the following reaction:

$$2A + B \leftrightarrow C$$

2 Problem Solution

2.1 P11-2_A

$$r_A = k(C_A - \frac{C_B}{K_C}) = 0 \tag{1}$$

$$C_A = C_{A0}(1-X), C_B = C_{A0}X \tag{2}$$

$$r_A = k(C_{A0}(1-X) - \frac{C_{A0}X}{K_C}) = 0 at X = X_e \tag{3}$$

$$(1-X_e) = \frac{X_e}{K_C} \tag{4}$$

$$K_C = \frac{X_e}{1-X_e} \tag{5}$$

$$K_C(T_2) = K_C(T_1) exp\left[\frac{\Delta H^o_{Rx}}{R} \times \left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right] \tag{6}$$

$$\frac{X_{e_2}}{1-X_{e_2}} = \frac{X_{e_1}}{1-X_{e_1}} exp\left[\frac{\Delta H^o_{Rx}}{R} \times \left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right] \tag{7}$$

$$\Delta H^o_{Rx} = -23.05 \text{kJ/mol} \tag{8}$$

2.2 Question 2

$$\Delta H_R(T) = H^o_{Rx}(T_R) + \int_{T_R}^{T} (C_P)_{prod} dT - \int_{T_R}^{T} (C_P)_{react} dT \tag{9}$$

$$\Delta H_R(T) = H^o_{Rx}(T_R) + \int_{T_R}^{T} (C_P)_C dT - \int_{T_R}^{T} (C_{P_B} + 2C_{P_A}) dT \tag{10}$$

$$ln \frac{K_C(T)}{K_C(T_1)} = \frac{\Delta H_R(T)}{R} \left(\frac{1}{T_1} - \frac{1}{T} \right) \tag{11}$$

$$= \frac{H^o_{Rx}(T_R) + \int_{T_R}^{T} (C_P)_C dT - \int_{T_R}^{T} (C_{P_B} + 2C_{P_A}) dT}{R} \left(\frac{1}{T_1} - \frac{1}{T} \right) \tag{12}$$