A. Review

1. Kinetic view of equilibrium: forward rate = backward rate
   \[ k_a = \frac{1}{k_i} = \frac{[C_i]}{[C_i]} \]

2. Thermodynamic view of equilibrium
   a. \( \Delta G^\circ \text{rxn} = -RT \ln K_{eq} \)
   b. \( \Delta G^\circ \text{rxn} \) and \( K_{eq} \) independent of pressure
   c. \( G = H - TS; \) \( dG = -SdT + VdP \)
   d. \( a_i = \text{activity coefficient} = \frac{\Pi}{P_i} \) for ideal gases
   e. Table available for \( \Delta G^\circ \text{rxn} \)
   f. \( K_y = K_y, P_{tot} = K_{tot} \) are dependent on total pressure if \( \Delta n = 0, \) but they compensate for each other so \( K_{eq} \) is independent of pressure!
   g. Given \( K_{eq} \) and \( P_{tot}, \) we can find \( y_i \)'s @ equilibrium if we have \( y_{feed} \) (one reaction only)

\[ K_{eq} = \frac{a_i^\alpha_i}{\Pi_i} \]

\[ K_{eq} = K_y \cdot K_{P_{tot}} = K_y \cdot \Pi_i \]

\[ K_{eq} = \sum_{i=1}^{n} y_i^\alpha_i \]

\[ \Delta G_{\text{react}}^\circ = \alpha_i \Delta G_{f_i} \]

\[ K_{eq} = K_y \cdot K_{P_{tot}} = K_y \cdot \Pi_i \]

\[ K_{eq} = \sum_{i=1}^{n} y_i^\alpha_i \]

\[ \Delta G_{\text{react}}^\circ = \sum_{i=1}^{n} \alpha_i \Delta G_{f_i} \]

B. More Concepts on equilibrium

• Hand-written notes…

C. Code Inputs

• \( Z_i \) low T range coefficients 300-1000 K
• \( Z_i \) high T range coefficients 1000-5000 K

\[ \frac{\delta^e_i}{P} = \left( \sum_{i=1}^{l} \frac{\delta_i^e \cdot T_i^e}{i} \right) \frac{T_i}{T} \]

\[ \frac{\delta^S_i}{P} = \left( \sum_{i=1}^{l} \frac{\delta_i^S \cdot T_i^e}{i} \right) \frac{T_i}{T} \]

• for ideal gas, \( C_p - C_v = R \)
• \( dH = C_p \ dT \) (i.e., no pressure dependence for ideal gas)
• \( dS = C_v \ dT \)
• \( dU = C_v \ dT \)

Approach

• Given expression for \( H_i^\circ(T) \) and \( S_i^\circ(T) \)

Get \( S_i \)

\[ S_i - S_i^0 = \int_{T_i}^{T} -R \ d\ln P \]

Get \( S \) and \( H \)

\[ S = \sum_i n_i S_i \]

\[ H = \sum_i n_i H_i \]

get \( G = H - TS \)

minimize \( G \)

Sample Input Thermo Data

• (from NASA-Lewis)