Example Equilibrium Calculation

- Given mixture of CO₂, CO, O₂ at specified T and p
- What is chemical composition?
  \[ \text{CO}_2 \leftrightarrow \text{CO} + \frac{1}{2} \text{O}_2 \]
- 3 unknowns require 3 equations

1) \[ K_p = \frac{P_{\text{CO}}P_{\text{O}_2}^{1/2}}{P_{\text{CO}_2}} = e^{\frac{\Delta G^{\circ}}{RT}} = \Pi K^0_j = \frac{K_{p_{\text{CO}_2}}^{1/2}}{K_{p_{\text{CO}}}^{1/2}} \]

2) \[ n^C = n_{\text{CO}} + n_{\text{CO}_2} = \frac{n_{\text{CO}} + n_{\text{CO}_2}}{n_{\text{CO}} + 2n_{\text{CO}_2} + 2n_{\text{O}_2}} = \frac{\chi_{\text{CO}} + \chi_{\text{CO}_2}}{\chi_{\text{CO}} + \chi_{\text{CO}_2} + 2\chi_{\text{O}_2}} \]

3) \[ n^O = n_{\text{CO}} + 2n_{\text{CO}_2} + 2n_{\text{O}_2} \quad \chi_{\text{CO}} + \chi_{\text{CO}_2} + \chi_{\text{O}_2} = 1 \]

Results CO/O₂/CO₂

- CO₂ is “low chemical energy” species
- Increasing O/C shifts composition from CO to CO₂
Results CO/O₂/CO₂

- Increasing pressure drives composition to CO₂
- At temperature extremes, weak pressure dependence