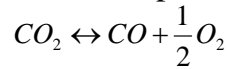


Example Equilibrium Calculation

- Given mixture of CO₂, CO, O₂ at specified *T* and *p*
- What is chemical composition? *must also specify atomic ratios*



- 3 unknowns require 3 equations

$$1) \quad K_p = \frac{p_{\text{CO}} p_{\text{O}_2}^{1/2}}{p_{\text{CO}_2}} = e^{-\frac{\Delta \hat{G}_R}{RT}} = \prod K_{p_{f,i}}^{\nu_i} = \frac{K_{p_{f,\text{CO}}} K_{p_{f,\text{O}_2}}^{1/2}}{K_{p_{f,\text{CO}_2}}}$$

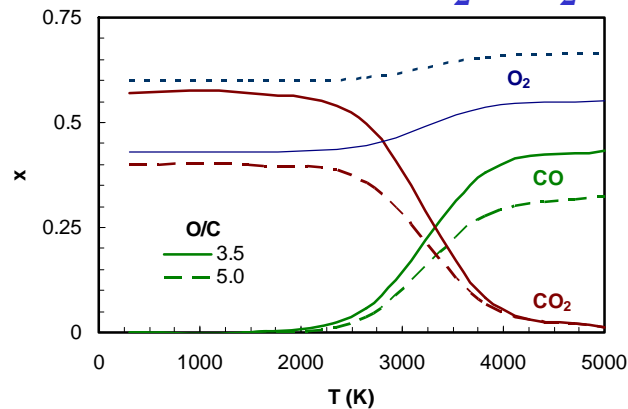
$$2) \quad n^c = n_{\text{CO}} + n_{\text{CO}_2} \quad \left(\frac{n^c}{n^o} \right) = \frac{n_{\text{CO}} + n_{\text{CO}_2}}{n_{\text{CO}} + 2n_{\text{CO}_2} + 2n_{\text{O}_2}} = \frac{\chi_{\text{CO}} + \chi_{\text{CO}_2}}{\chi_{\text{CO}} + 2\chi_{\text{CO}_2} + 2\chi_{\text{O}_2}}$$

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

Chem Equil. Example 1
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Results CO/O₂/CO₂

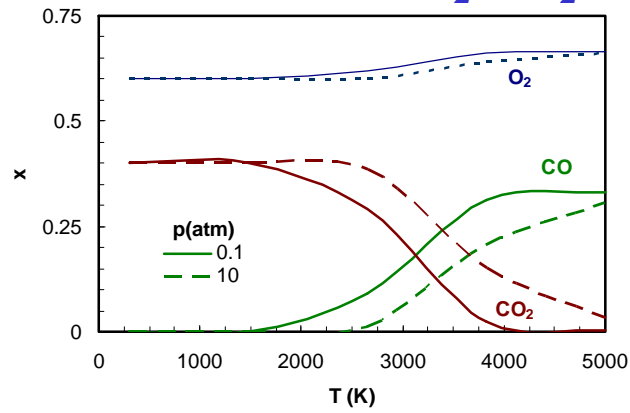


- CO₂ is “low chemical energy” species
- Increasing O/C shifts composition from CO to CO₂

Chem Equil. Example 2
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Results CO/O₂/CO₂



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