**Example Equilibrium Calculation**

- Given mixture of CO$_2$, CO, O$_2$ at specified $T$ and $p$
  - what is chemical composition (e.g., $n_i$ or $\chi_i$)?
- Can write chemical state relation ("reaction")
  \[ CO_2 \leftrightarrow CO + \frac{1}{2} O_2 \]

1) \[ K_p = \frac{p_{CO}^{1/2}}{p_{CO_2}} = \frac{\chi_{CO}^{1/2}}{\chi_{CO_2}} p^{1/2} = e^{\frac{\Delta G_k}{RT}} = \Pi K_{i,j} = \frac{K_{P,f,CO}}{K_{P,f,O_2}} \]

- But 3 unknowns requires 3 equations
  - can write atom balances (mass conservation), 1 for each nuclei type

2) \[ n^C = n_{CO} + n_{CO_2} \quad n_i^{mass} = n_{CO} + 2n_{CO_2} + 2n_{O_2} \]

3) \[ n^O = 2n_{CO} + 2n_{CO_2} + 2n_{O_2} \quad \chi_{CO} + 2\chi_{CO_2} + 2\chi_{O_2} = 1 \]

**Results CO/O$_2$/CO$_2$**

- CO$_2$ is “low chemical energy” species
- Increasing O/C shifts composition from CO to CO$_2$
• Increasing pressure drives composition to CO$_2$
• At temperature extremes, weak pressure dependence