2005 Controls II #2

(2) (a) $Ca^{2+}/O^{2-}, SiO_4^{4-}, S^{2-}$

$$\begin{cases} n_{Ca^{2+}} = (X_{CaO} + X_{CaS}) \\ n_{S^{2-}} = X_{CaS} \\ n_{SiO_4^{4-}} = X_{SiO_2} \\ n_{O^{2-}} = (X_{CaO} - 2X_{SiO_2}) \end{cases} \qquad \begin{cases} X_{Ca^{2+}} = 1 \\ X_{O^{2-}} = \dfrac{X_{CaO} - 2X_{SiO_2}}{X_{CaO} - X_{SiO_2} + X_{CaS}} \\ X_{S^{2-}} = \dfrac{X_{CaS}}{X_{CaO} - X_{SiO_2} + X_{CaS}} \end{cases}$$

$$a_{CaO} = X_{Ca^{2+}} X_{O^{2-}} = \frac{X_{CaO} - 2X_{SiO_2}}{X_{CaO} - X_{SiO_2} + X_{CaS}} \quad (1)$$

$$a_{CaS} = X_{Ca^{2+}} X_{S^{2-}} = \frac{X_{CaS}}{X_{CaO} - X_{SiO_2} + X_{CaS}} \quad (2)$$

(b) Exchange of O and S between gas and slag

$$\tfrac{1}{2}O_2 + CaS = \tfrac{1}{2}S_2 + CaO \qquad \Delta g^\circ = \left(g^\circ_{CaO} + \tfrac{1}{2}g^\circ_{S_2} - \tfrac{1}{2}g^\circ_{O_2} - g^\circ_{CaS}\right) \quad (3)$$

$$\Delta g^\circ = -RT \ln K \quad (4)$$

$$K = \left(\frac{P_{S_2}}{P_{O_2}}\right)^{1/2} \cdot \frac{a_{CaO}}{a_{CaS}} = \left(\frac{P_{S_2}}{P_{O_2}}\right)^{1/2} \frac{(X_{CaO} - 2X_{SiO_2})}{X_{CaS}}$$

Substitute Eqs. (1), (2), (3), (4) to give X_{CaS} as a function of

Δg°, P_{O_2}, P_{S_2}, T, X_{CaO}, X_{SiO_2}