Derive the concentration profile for $F_{2(g)}$ reacting with a U sphere to produce $UF_{6(g)}$ by the reaction

$$3F_{2\,(g)} + U_{(s)} = UF_{6\,(g)}$$

Assume the U is intermingled with fine particles of Al_2O_3 that form a porous layer of alumina through which the above gases diffuse. Use the following BC's: at $r=r_o$, $X_{F2}=X^o$ and at $r=r_1$, $X_{F2}=1$.

Solution

First determine the form of Fick's Law including the bulk diffusion terms.

$$N_{F_2} = X_{F_2}\left(N_{F_2} + N_{UF_6}\right) - C\mathcal{D}_{F_2,UF_6}\frac{\partial X_{F_2}}{\partial r} \qquad \text{text Eq. (14.4)}$$

$$N_{F_2} = -3N_{UF_6} \qquad (1)$$

$$N_{F_2} = -\frac{C\mathcal{D}_{F_2,UF_6}}{\left(1-\frac{2}{3}X_{F_2}\right)}\frac{\partial X_{F_2}}{\partial r} \qquad (2)$$

$$N_{F_2} = \frac{3C\mathcal{D}_{F_2,UF_6}}{2}\frac{\partial \ln\left(1-\frac{2}{3}X_{F_2}\right)}{\partial r} \qquad (3)$$

Second, write the known relationship for the change of a flux in spherical coordinates at steady state.

$$\frac{\partial\left(r^2 N_{F_2}\right)}{\partial r} = 0 \qquad (4)$$

Substitute in Fick's Law

$$\frac{\partial\left(r^2\frac{3C\mathcal{D}_{F_2,UF_6}}{2}\frac{\partial \ln\left(1-\frac{2}{3}X_{F_2}\right)}{\partial r}\right)}{\partial r} = 0 \qquad (5)$$

Rearrange and integrate once, indefinitely.

$$\left(\frac{r^2\partial \ln\left(1-\frac{2}{3}X_{F_2}\right)}{\partial r}\right) = C_1 \qquad (6)$$

Integrate again to obtain

$$\ln\left(1-\frac{2}{3}X_{F_2}\right)=-\frac{C_1}{r}+C_2 \tag{7}$$

Apply the BC's.

$$\ln\left(1-\frac{2}{3}X_{F_2}^{\circ}\right)=-\frac{C_1}{r_{\circ}}+C_2 \tag{8}$$

$$\ln\left(\frac{1}{3}\right)=-\frac{C_1}{r_1}+C_2 \tag{9}$$

Solve for C_1 and C_2.

$$C_1=\frac{\ln\left(3-2X_{F_2}^{\circ}\right)}{\left[\frac{1}{r_1}-\frac{1}{r_{\circ}}\right]} \tag{10}$$

$$C_2=-\frac{C_1}{r_1}-\ln\left(\frac{1}{3}\right) \tag{11}$$

Substituting into Eq (8) gives

$$\ln\left(1-\frac{2}{3}X_{F_2}\right)=-\frac{\ln\left(3-2X_{F_2}^{\circ}\right)}{\left[\frac{1}{r_1}-\frac{1}{r_{\circ}}\right]}\left(\frac{1}{r}-\frac{1}{r_1}\right)+\ln\left(\frac{1}{3}\right), \tag{12}$$

which may be written in dimensionless form as

$$\frac{\ln\left(3-2X_{F_2}\right)}{\ln\left(3-2X_{F_2}^{\circ}\right)}=-\frac{\left[\frac{1}{r}-\frac{1}{r_1}\right]}{\left[\frac{1}{r_1}-\frac{1}{r_{\circ}}\right]}. \tag{13}$$

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