Topic - Tutorial steady state molecular diffusion

A fluidized coal reactor has been proposed for a new power plant. If operated at 1145 K, the process will be limited by the diffusion of oxygen countercurrent to the carbon dioxide, CO_2, formed at the particle surface. Assume that the coal is pure solid carbon with a density of $1.28 \times 10^3 kg/m^3$ that the particle is spherical with an initial diameter of $1.5 \times 10^{-4}\, m(150\mu m)$. Air (21% O_2 and79% N_2) exists several diameters away from the sphere. Under the conditions of the combustion process, the diffusivity of oxygen in the gas mixture at 1145 K is $1.3 \times 10^{-4} cm^2/s$. If a steady-state process is assumed,

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calculate the time necessary to reduce the diameter of the carbon particle to $5 \times 10^{-5}\, m(50\mu m)$. The surrounding air serves as an infinite source for O_2 transfer, whereas the oxidation of the carbon at the surface of the particle is the sink for O_2 mass transfer. The reaction at the surface is:

$$C(s) + O_2(g) \rightarrow CO_2(g)$$

At the surface of the coal particle, the reaction is so rapid.

Solution:

The pure carbon particle is the source for the CO_2 flux and the sink for O_2 flux. As the coal particle is oxidized, there will be an output of carbon as stipulated by the stoichiometry of the reaction.

Number of moles of oxygen transferred = number of moles of carbon reacted

Number of moles transferred of oxygen = mole flux × area

$$Number\ of\ moles\ transferred\ of\ oxygen = N_{O_2-mix} \times 4\pi r^2$$

N_{O_2-mix} can be obtained by using the general differential equation with the Fick's equation as follows:

By applying the following assumptions on the general differential equation of mass transfer:

$$\nabla.\vec{N}_A + \frac{\partial c_A}{\partial t} - R_A = 0$$

1. Steady state oxygen diffusion
2. One dimensional mass transfer in r direction
3. No homogenous reaction
4. Instantaneous heterogeneous reaction

$$\therefore \nabla.\vec{N}_A = 0$$

For diffusion of oxygen in r-direction

$$\frac{1}{r^2}\frac{d}{dr}(r^2 N_{O_2}) = 0$$

$$\therefore \frac{d}{dr}(r^2 N_{O_2}) = 0$$

The above equation specifies that $r^2 N_{O_2}$ is constant over the diffusion path in the r direction, so that

$$r^2 N_{O_2}\Big|_r = R^2 N_{O_2}\Big|_R$$

Form Fick's equation:

$$N_{O_2} = -cD_{O_2-mix}\frac{dy_{O_2}}{dr} + y_{O_2}(N_{O_2} + N_{CO_2})$$

But from the stoichiometry of the reaction

$$N_{O_2} = -N_{CO_2}$$

i.e. equimolar counter diffusion

$$\therefore N_{O_2} = -cD_{O_2-mix}\frac{dy_{O_2}}{dr}$$

$$N_{O_2}\int_R^{\infty} dr = -cD_{O_2-mix}\int_0^{y_{O_2,\infty}} dy_{O_2}$$

$$N_{O_2} r^2 \int_R^{\infty} \frac{dr}{r^2} = -cD_{O_2-mix}\int_0^{y_{O_2,\infty}} dy_{O_2}$$

$$N_{O_2} r^2 \left(\frac{1}{R}\right) = -cD_{O_2-mix}(y_{O_2,\infty} - 0)$$

$$N_{O_2} r^2 = -RcD_{O_2-mix}\, y_{O_2,\infty}$$

$$number\ of\ moles\ of\ oxygen\ transfered\ per\ unit\ time = N_{O_2} \times 4\pi r^2$$

$$number\ of\ moles\ of\ oxygen\ transfered\ per\ unit\ time = -4\pi R\ cD_{O_2-mix}\, y_{O_2,\infty}$$

The negative sign because the transfer of oxygen is in the opposite direction of r

$$\therefore number\ of\ moles\ of\ carbon\ consumed\ \ per\ unit\ time = 4\pi R\ cD_{O_2-mix}\, y_{O_2,\infty}$$

By applying the law of conservation of mass on the carbon:

$$\text{Input} - \text{output} + \text{generation} - \text{consumption} = \text{accumulation(rate of change)}$$

$$-\text{consumption} = \text{accumulation(rate of change)}$$

$$-4\pi R\, cD_{O_2-mix}\, y_{O_{2,\infty}} = \frac{dN}{dt} = \frac{\rho_c}{M.wt}\frac{dV}{dt}$$

$$V = \frac{4}{3}\pi R^3$$

$$-4\pi R\, cD_{O_2-mix}\, y_{O_{2,\infty}} = \frac{\rho_c}{M.wt} 4\pi R^2 \frac{dR}{dt}$$

$$dt = -\frac{\rho_c}{M.wt}\frac{R\, dR}{cD_{O_2-mix}\, y_{O_{2,\infty}}}$$

by integrating the above equation between the limits:

$$at\ t = 0 \qquad R = R_i = 7.5 \times 10^{-5}\ m$$

$$at\ t = t \qquad R = R_f = 2.5 \times 10^{-5}\ m$$

$$\int_0^t dt = -\frac{\rho_c}{M.wt}\frac{1}{cD_{O_2-mix}\, y_{O_{2,\infty}}}\int_{R_i}^{R_f} R\, dR$$

$$t = \frac{\rho_c}{2\,M.wt}\frac{(R_i^2 - R_f^2)}{cD_{O_2-mix}\, y_{O_{2,\infty}}}$$

$$c = \frac{p}{RT} = 0.0106\ kmol/m^3$$

$$y_{O_{2,\infty}} = 0.21$$

$$\therefore t = 0.92\ s$$

References:

1. Kothandaraman C.P “Fundamentals of Heat and Mass Transfer” New Age International, New Delhi,4th Edition 2012 (Unit I, II, III, IV, V).
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3. MIT open courseware – https://ocw.mit.edu/courses/mechanical-engineering

Other web sources