External mass transfer coefficients in packed beds

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There are a variety of correlations of mass transfer coefficients available in the literature. From Perry's Chemical Engineers' Handbook, 6th ed., p. 4-38 (1984), the Chilton-Colburn correlations can be expressed in the following manner. The mass transfer coefficient for species A in a gas, k_{gA}, is given by:

$$k_{gA}\left[\frac{mol}{s \cdot m^2 \cdot Pa}\right] = 0.99\left(\frac{G}{\bar{M}P_{fa}}\right)\text{Sc}^{-2/3}\,\text{Re}^{-0.41} \quad \text{for Reynolds number} > 350$$

$$k_{gA}\left[\frac{mol}{s \cdot m^2 \cdot Pa}\right] = 1.82\left(\frac{G}{\bar{M}P_{fa}}\right)\text{Sc}^{-2/3}\,\text{Re}^{-0.51} \quad \text{for Reynolds number} < 350$$

See below for explanation of these correlations in terms of Chilton-Colburn j_D factors.

Reynolds number: $$\text{Re} \equiv \frac{d_p G}{\mu} = \frac{\text{momentum convection}}{\text{momentum diffusion}}$$

Schmidt number: $$\text{Sc} \equiv \frac{\mu}{\rho_f D_A} = \frac{\text{momentum diffusion}}{\text{mass diffusion}}$$

Superficial mass velocity: $$G\left[\frac{kg}{m^2 s}\right] = \frac{\dot{m}}{A_x}$$

Reactor cross-sectional area: $$A_x\left[m^2\right] = \pi\left(\frac{d_{rxr}}{2}\right)^2$$

Pressure film factor: $$P_{fa} = P_{total} + P_A\delta_A$$

The Schmidt number and the Reynolds number are dimensionless, $\bar{M}$ is mean molecular weight of the gas (kg/mol), d_p is catalyst pellet diameter (m), μ is fluid viscosity (Pa · s = kg/s/m), ρ_f is gas density (kg/m^3), D_A is the diffusion coefficient of A (m^2/s) in the gas mixture, $\dot{m}$ is mass flow rate into reactor (kg/s), d_{rxr} is the internal diameter of the reactor vessel (m), P_{total} is the gas total pressure (Pa), P_A is the partial pressure of reactant species A (Pa), and δ_A is the change in moles with reaction per mole species A ((moles products minus moles reactants) / moles A).

The rate of mass transfer rate of species A from the bulk gas to the external surface of catalyst pellets is given by:

$$r_A\left[\frac{mol}{kg\cdot s}\right]=a_{es}\left[\frac{m^2}{kg}\right]k_{Ag}\left[\frac{mol}{s\cdot m^2\cdot Pa}\right]\left(P_{A,bulk}\left[Pa\right]-P_{A,es}\right)$$

$$r_A\left[\frac{mol}{kg\cdot s}\right]=a_{es}\left[\frac{m^2}{kg}\right]k_{Ag}\left[\frac{mol}{s\cdot m^2\cdot Pa}\right]R_g\left[\frac{Pa\cdot m^3}{mol\cdot K}\right]T\left[K\right]\left(C_{A,bulk}\left[\frac{mol}{m^3}\right]-C_{A,es}\right)$$

$$r_A\left[\frac{mol}{kg\cdot s}\right]=a_{es}\left[\frac{m^2}{kg}\right]k_m\left[\frac{m}{s}\right]\left(C_{A,bulk}\left[\frac{mol}{m^3}\right]-C_{A,es}\right)$$

$$k_m\left[\frac{m}{s}\right]=k_{Ag}\left[\frac{mol}{s\cdot m^2\cdot Pa}\right]R_g\left[\frac{Pa\cdot m^3}{mol\cdot K}\right]T\left[K\right]$$

External surface area of pellets: $a_{es}\left[\frac{m^2}{kg}\right]=\frac{4\pi\left(d_p/2\right)^2}{\rho_p\left(4/3\right)\pi\left(d_p/2\right)^3}=\frac{6}{\rho_p d_p}$

The subscript "es" refers to conditions at the external surface of the pellets and ρ_p is the pellet density (kg/m^3),

The correlations for k_{gA} given above are from rearrangement of the Chilton-Colburn j_D factor correlations

$$k_{gA}\left[\frac{mol}{s\cdot m^2\cdot Pa}\right]=0.99\left(\frac{G}{\bar{M}P_{fa}}\right)\mathrm{Sc}^{-2/3}\,\mathrm{Re}^{-0.41}\qquad \text{for Re} > 350$$

This can be expressed as

$$j_D=\left(\frac{k_{gA}\bar{M}P_{fa}}{G}\right)\mathrm{Sc}^{2/3}=\frac{\mathrm{Sh}}{\mathrm{Sc}^{1/3}\,\mathrm{Re}}=0.99\,\mathrm{Re}^{-0.41}$$

Sherwood number: $\mathrm{Sh}\equiv\frac{k_m\left[\frac{m}{s}\right]d_p\left[m\right]}{D_A\left[\frac{m^2}{s}\right]}$

Note that the Chilton-Colburn j_D factor is a function of Reynolds number only.

The correlation can also be expressed as:

$$\text{Sh} = 0.99\text{Sc}^{1/3}\,\text{Re}^{0.59} \qquad \text{for Re} > 350$$

The Sherwood number is a dimensionless mass transfer coefficient and can also be considered a dimensionless concentration gradient. It is also referred to as the Nusselt number for mass transfer.