25 Mar 19
FAM
(9Am)

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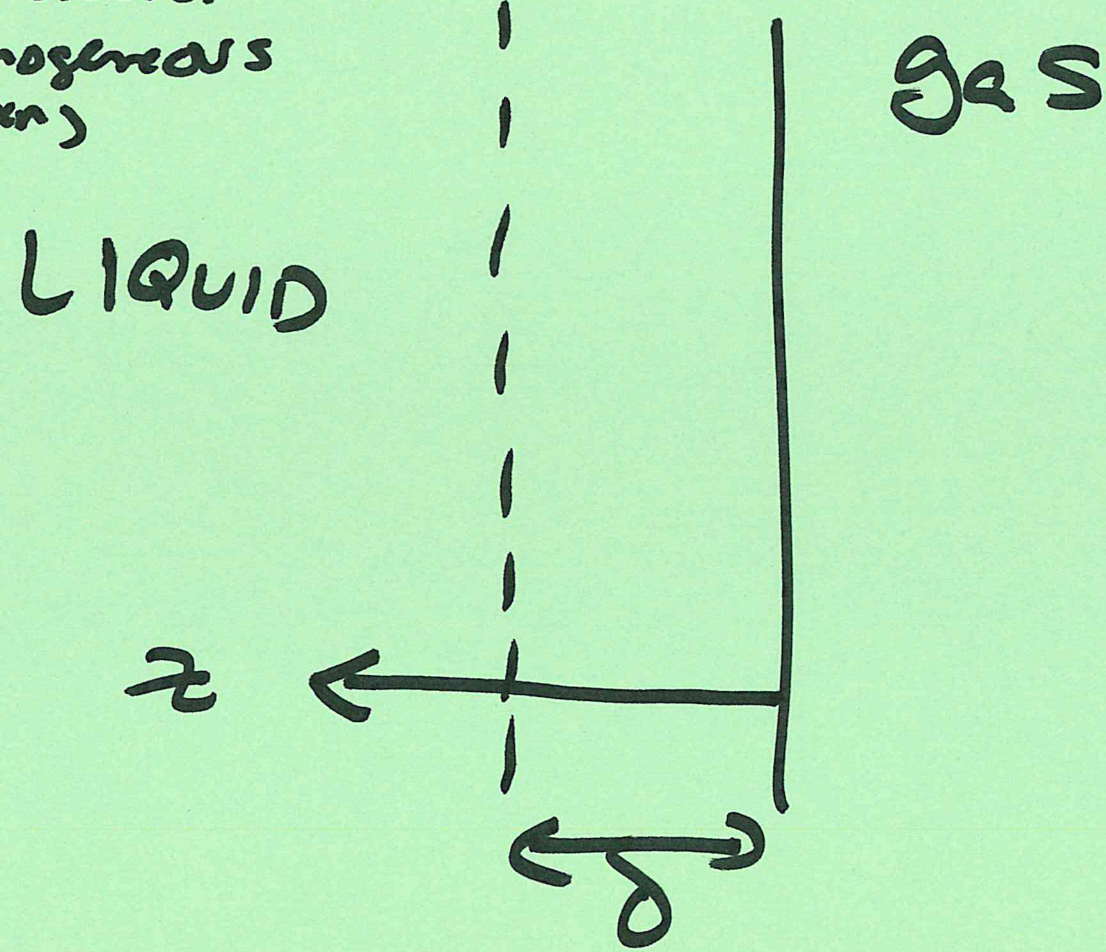
Example 5:

Gas Absorption

(diffusion w/ homogeneous rxn)



(penetration theory)

We will use N_{Az} mass species A bal since we have chemical rxn

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The Equation of Species Mass Balance in Terms of Combined Molar quantities in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B.

The general case, where the combined molar flux with respect to molar velocity ($\underline{N}_A$), is given on page 1.

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In terms of total molar flux, $\underline{N}_A$

Microscopic species mass balance, in terms of molar flux; Gibbs notation

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

Microscopic species mass balance, in terms of combined molar flux; Cartesian coordinates

steady

$$\cancel{\frac{\partial c_A}{\partial t}} = -\left(\cancel{\frac{\partial N_{A,x}}{\partial x}} + \cancel{\frac{\partial N_{A,y}}{\partial y}} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; cylindrical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{A,r})}{\partial r} + \frac{1}{r}\frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

$$0 = \frac{dN_{Az}}{dz} + R_A$$

Microscopic species mass balance, in terms of combined molar flux; spherical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{A,r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{A,\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{A,z}}{\partial \phi}\right) + R_A$$

one dimensional

Fick's law of diffusion, Gibbs notation: $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

$$= c_A\underline{v}^* - cD_{AB}\nabla x_A$$

Fick's law of diffusion, Cartesian coordinates:

$$\begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} \cancel{x_A(N_{A,x} + N_{B,x}) - cD_{AB}\frac{\partial x_A}{\partial x}} \\ \cancel{x_A(N_{A,y} + N_{B,y}) - cD_{AB}\frac{\partial x_A}{\partial y}} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$$

stagnant

Fick's law of diffusion, cylindrical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,z} \end{pmatrix}_{r\theta z} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$$

Fick's law of diffusion, spherical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

Species A mass Bal:

$$0 = -\frac{dN_{Az}}{dz} + R_A$$

$$R_A = -k_1 C_A$$

$$0 = -\frac{dN_A}{dz} - k_1 C_A$$

<u>Fick's Law</u>
$(N_{Bz}=0)$

$$N_{Az} - x_A N_{Az} = -c D_{AB} \frac{dx_A}{dz}$$

☆ if A is <u>dilute</u>:

$$\begin{cases} 1 - x_A \approx 1 \\ c\,\dfrac{dx_A}{dz} = dC_A/dz \end{cases}$$

Fick's Law (con't)

$$N_{Az}(1 - x_A) = -c\,D_{AB}\,\frac{dx_A}{dz}$$

using the dilute assumption:

$$N_{Az} = -D_{AB}\,\frac{dc_A}{dz}$$

Substituting into species A mass bal:

$$0 = \frac{d}{dz}\left(-D_{AB}\,\frac{dc_A}{dz}\right) + k_1 c_A$$

constant D_{AB}

$$\boxed{0 = -D_{AB}\frac{d^2C_A}{dz^2} + k_1 C_A}$$

Second-order ordinary differential equation (ODE) with constant coefficients.

(classic form; soln is sum of cosh + sinh functions; see WRF p 505)

BC: (penetration model)

$$\boxed{\begin{array}{ll} z = 0 & C_A = C_{A0} \\ z = \delta & C_A = 0 \end{array}}$$

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