4-MAR 2019
FAM

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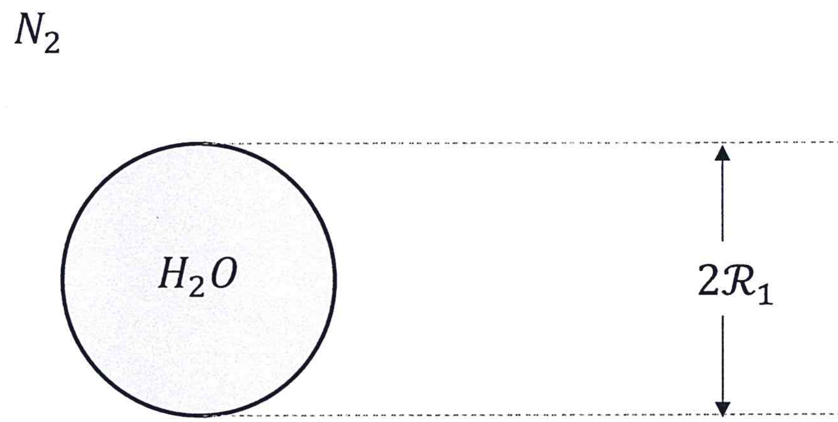
QUICK START

Example: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). What is the water mole fraction as a function distance from the droplet?



Let's Interrogate the problem.

DROPLET : 2

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

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

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

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

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

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

no homogeneous rxn

steady state

θ, ϕ symmetry

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:

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

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:

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

B is stagnant (no sink)

<u>microscopic species A mass balance</u>

$$0 = \cancel{-\frac{1}{r^2}}\frac{d}{dr}(\underbrace{r^2 N_{A,r}}_{\equiv \Phi})$$

$$\frac{d\Phi}{dr} = 0$$

$$\Phi = C_1$$

$$r^2 N_{A,r} = C_1$$

$$\boxed{N_{A,r} = \frac{C_1}{r^2}}$$

From before $\boxed{N_{Ar} = \frac{c_1}{r^2}}$

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<u>Ficks</u> <u>Law of Diffusion:</u>

$$N_{Ar} = x_A N_{Ar} - c D_{AB} \frac{dx_A}{dr}$$

$$\frac{c_1}{r^2} \rightarrow N_{Ar} (1 - x_A) = - c D_{AB} \frac{dx_A}{dr}$$

$$\frac{c_1}{r^2} dr = - c D_{AB} \frac{dx_A}{(1 - x_A)}$$

$$\int \left(\frac{-c_1}{c D_{AB}}\right) r^{-2} dr = (-1) \int \frac{-dx_A}{\underbrace{(1 - x_A)}_{= u}}$$

$du = -dx_A$

$$\left(\frac{+c_1}{c D_{AB}}\right) \frac{r^{-1}}{+1} = -\ln(1 - x_A) + c_2$$

BC: $r = R_1 \quad x_A = x_A^*$ (saturated)

two possible choices

$r = \infty \quad x_A = x_{A\infty}$ ← isolated drop

or

$r = R_2 \quad x_A = x_{A2}$ ← FILM model

<u>Solve</u> (we use BC #2)

⋮

1. substitute
2. 2 eqns, 2 unknowns
3. algebra

$$\Rightarrow \boxed{c_1 = c D_{AB} \frac{\ln\left(\frac{1-x_{A1}}{1-x_{A2}}\right)}{\frac{1}{R_2} - \frac{1}{R_1}}}$$

$c_2 =$

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$$\boxed{C_2 = \ln(1-X_{A1}) + \left(\frac{\frac{1}{R_1}}{\frac{1}{R_2} - \frac{1}{R_1}}\right) \ln\left(\frac{1-X_{A1}}{1-X_{A2}}\right)}$$

substitute back ...

Final result:

dependent variable

indep variable

$$\boxed{\left(\frac{1-X_{A2}}{1-X_{A1}}\right)^{\left(\frac{1/R_1 - 1/r}{1/R_1 - 1/R_2}\right)} = \frac{(1-X_A)}{(1-X_{A1})}}$$

(compare WRF p502)

$X_A(r)$ //

FINAL MODEL

(8)

QUICK START

Example: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the water mole fraction in the film as a function of radial position? You may assume ideal gas properties for air.