1D Radial Diffusion

24 Feb 2021 CM3120 F. MORRISON 0

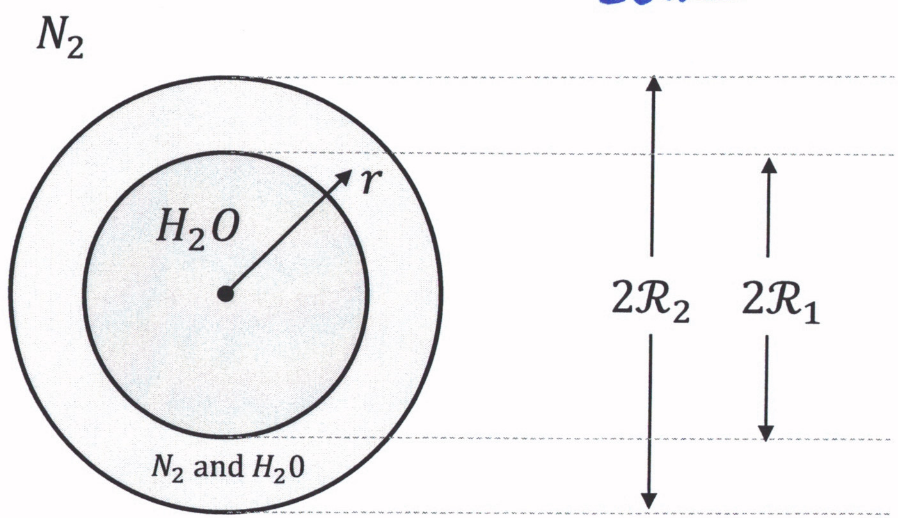
PART 6

QUICK START

**Example 2**: 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 rate of evaporation and how does the water concentration vary in the gas as a function distance from the droplet? You may assume ideal gas properties for air.

$x_{bulk}$

See HW Plms 3.14 3.8




We are developing a *model* to address the questions of interest

BC: $r = \mathcal{R}_1 \quad x_A = \dfrac{P^*}{P}$

$r = \mathcal{R}_2 \quad x_A = x_{bulk}$

Ver 2

BSL2, p550

0.5

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.

**Spring 2019 Faith A. Morrison, Michigan Technological University**

---

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

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

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

WRF 25-11

**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

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

Steady

$\theta$ $\phi$ Symmetry

no rxn

---

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

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

WRF 24-22

**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:

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

---

EXAMPLE 2: Water droplet ①

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

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

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

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

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.

**Spring 2019 Faith A. Morrison, Michigan Technological University**

---

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

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

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A \qquad \text{WRF 25-11}$$

**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

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

---

**Fick's law of diffusion**, Gibbs notation: $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$ WRF 24-22

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

TRANSPORT LAW:

**Fick's law of diffusion**, Cartesian coordinates:

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

Stagnant B

**Fick's law of diffusion**, cylindrical coordinates:

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

$N_{Br} = 0$

**Fick's law of diffusion**, spherical coordinates:

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

stagnant

$$N_{A,r} = x_A N_{A,r} - c\mathcal{D}_{AB}\,\frac{dx_A}{dr}$$

$$N_{A,r}(1-x_A) = -c\mathcal{D}_{AB}\,\frac{dx_A}{dr}$$

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

$$\frac{c_1}{r^2}(1-x_A) = -c\mathcal{D}_{AB}\,\frac{dx_A}{dr}$$

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

$$\left(\cancel{-}\frac{c_1}{c\mathcal{D}_{AB}}\right)\frac{r^{-1}}{\cancel{-}1} = -\ln(1-x_A) + C_2$$

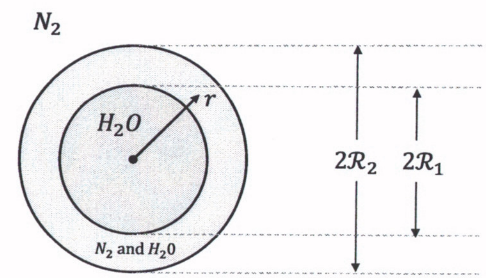
Solution:

1. apply BC
2. 2 eqns, 2 unknowns, solve for $C_1$, $C_2$
3. Substitute back. Obtain:
   - $N_{Ar}$
   - $x_A(r)$

QUICK START

Ver 2

**Example 2**: 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 rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.




Ver 2

Assumptions:

- Steady diffusion; stagnant air
- Uniform film surrounds droplet
- Ideal gas
- Constant temperature and pressure
- Constant $c, \mathcal{D}_{AB}$

**Solution:**

$x_A(r)$

$$\frac{1-x_A}{1-x_{A1}} = \left(\frac{1-x_{A2}}{1-x_{A1}}\right)^{\left(\frac{\frac{1}{\mathcal{R}_1}-\frac{1}{r}}{\frac{1}{\mathcal{R}_1}-\frac{1}{\mathcal{R}_2}}\right)}$$

See HW 3.14
3.8

Homework problem 3.8: plot this solution

BSL2, p550