

CM3120: Module 3

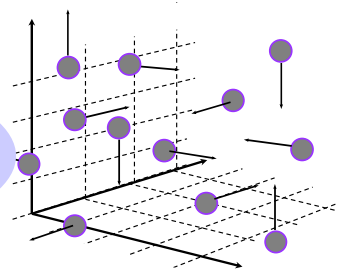
Diffusion and Mass Transfer I

- I. Introduction to diffusion/mass transfer
- II. Classic diffusion and mass transfer—Quick Start a): 1D Evaporation
- III. Classic diffusion and mass transfer—Quick Start b): 1D Radial droplet
- IV. Cycle back: Fick's mass transport law
- V. Microscopic species A mass balance
- VI. Classic diffusion and mass transfer—c): 1D Mass transfer with chemical reaction

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CM3120: Module 3

Module 3 Lecture III Quick Start 2: 1D Radial Diffusion



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www.chem.mtu.edu/~fmorriso/cm3120/cm3120.html

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Diffusion and Mass Transfer

It turns out that there are many interesting and applicable problems we can address readily with **this** form of the species mass balance.

Microscopic species mass balances—**a time**

In terms of **species** $\frac{d}{dt} \int_V c_i dV + \int_V \nabla \cdot (c_i \mathbf{v}_i) dV = \int_V \dot{c}_i dV$

In terms of **species** $\frac{d}{dt} \int_V c_i dV + \int_V \nabla \cdot (c_i \mathbf{v}_i) dV = \int_V \dot{c}_i dV$

In terms of **species** $\frac{d}{dt} \int_V c_i dV + \int_V \nabla \cdot (c_i \mathbf{v}_i) dV = \int_V \dot{c}_i dV$

Let's jump in!


Microscopic species mass balance in terms of combined molar flux N_i .

We'll do a "Quick Start" and get into some examples and return to the "why" of it all a bit later.

CM3120 Transport/Unit Operations 2

Diffusion and Mass Transfer


in MIXTURES




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QUICK START


(to problem solving)



Continuing...



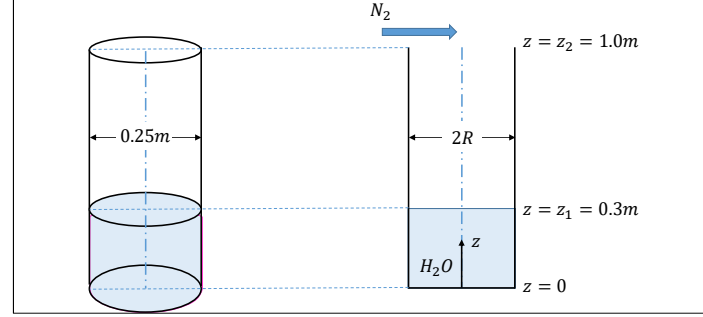
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Last time...


QUICK START

Example 1: Water (40°C, 1.0 atm) slowly and steadily evaporates into nitrogen (40°C, 1.0 atm) from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. **What is the rate of water evaporation?**



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Last time...

Interrogating the problem:

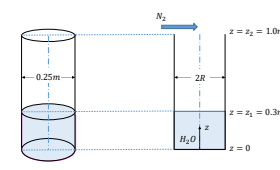
Why does the water evaporate?

What limits the rate of evaporation?

What could be done to accelerate the evaporation?


What could be done to slow down the evaporation?

Example: Water (40°C , 1.0 atm) slowly and steadily evaporates into nitrogen (40°C , 1.0 atm) from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02 . **What is the rate of water evaporation?**



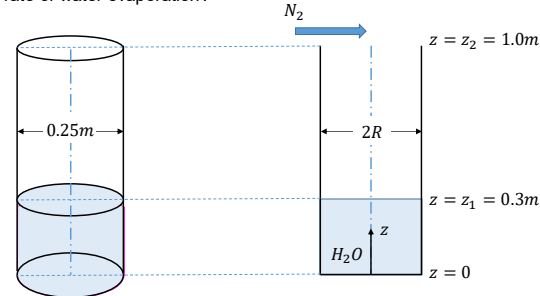
We take note of the questions that were productive in leading us to the solution.

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Last time...

Example 1: Water (40°C , 1.0 atm) slowly and steadily evaporates into nitrogen (40°C , 1.0 atm) from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02 . **What is water mole fraction as a function of vertical position in the tank? You may assume ideal gas properties. What is the rate of water evaporation?**



The questions led us to **refine the problem**; to frame it in a way that led to the solution.

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Example 1

Seek concentration distribution
 ⇒ microscopic species A mass balance.

The Equation of Species Mass Balance in Terms of **combined** **flux** quantities in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. The general case, where the **combined** flux with respect to molar velocity (\bar{c}_A) is given in page 8. Spring 2010 Faith A. Morrison, Michigan Technological University

Microscopic species mass balance, in terms of radial flux, Gibbs notation

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

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

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

Fick's law of diffusion, Gibbs notation: $N_A = -c_1 D_{AB} \nabla^2 x_A$

Fick's law of diffusion, Cartesian coordinates: $N_A = -c_1 D_{AB} \frac{dx_A}{dz}$

Fick's law of diffusion, cylindrical coordinates: $N_A = -c_1 D_{AB} \left(\frac{dx_A}{dz} + x_A \frac{dx_A}{z} \right)$

Fick's law of diffusion, spherical coordinates: $N_A = -c_1 D_{AB} \left(\frac{dx_A}{dz} + \frac{2x_A}{z} \right)$

Handwritten notes: "no r-dependence", "symmetry", "segment B"

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EXAMPLE 1: STEADY DIFFUSION FROM A CYLINDRICAL TANK

MICRO SPECIES "A" MASS BALANCE (cylindrical) see PS

$\frac{dN_{A,z}}{dz} = 0$

integrate: $N_{A,z} = C_1$

Fick's Law: (cylindrical) see PS

$N_{A,z} = x_A N_{A,z} - c_1 D_{AB} \frac{dx_A}{dz}$

$C_1 - x_A N_{A,z} = -c_1 D_{AB} \frac{dx_A}{dz}$

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Example 1

$N_{A,z}(1-x_A) = -c_1 D_{AB} \frac{dx_A}{dz}$ (3)

from species mass balance $\Rightarrow C_1 = N_{A,z}$

$N_{A,z} dz = -c_1 D_{AB} \frac{dx_A}{(1-x_A)}$

$\int C_1 dz = -c_1 D_{AB} \int \frac{dx_A}{(1-x_A)}$

$C_1 z = +c_1 D_{AB} \ln(1-x_A) + C_2$ *du = -dx_A*

BC: $z = z_2, x_A = 0, C_2 = N_{A,z} z_2$

$z = z_1, x_A = x_A^1, C_2 = N_{A,z} z_1$ *Results from*

To Solve:

- substitute
- obtain 2 equations, 2 unknowns
- solve for C_1, C_2

results:

$$\begin{cases} C_1 = \frac{c_1 D_{AB}}{(z_1 - z_2)} \ln \left(\frac{1-x_{A1}}{1-x_{A2}} \right) \\ C_2 = \ln(1-x_{A1}) - \frac{z_1}{(z_1 - z_2)} \ln \left(\frac{1-x_{A1}}{1-x_{A2}} \right) \end{cases}$$

- substitute back. Final answer:

$$\left(\frac{1-x_A}{1-x_{A1}} \right) = \left(\frac{1-x_{A1}}{1-x_{A2}} \right)^{\frac{(z-z_1)/(z_1-z_2)}{(z_1-z_2)/z_1}}$$

First, we obtained the flux $N_{A,z}$ and the concentration distribution $x_A(z)$.

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Example 1

To Solve:

- substitute
- obtain 2 equations, 2 unknowns
- solve for C_1, C_2

results:

$$C_1 = \frac{cD_{AB}}{(z_1 - z_2)} \ln \left(\frac{1 - X_{A1}}{1 - X_{A2}} \right)$$

$$C_2 = \ln(1 - X_{A1}) - \frac{z_1}{(z_1 - z_2)} \ln \left(\frac{1 - X_{A1}}{1 - X_{A2}} \right)$$

- substitute back. Final answer:

$$\left(\frac{1 - X_{A1}}{1 - X_{A2}} \right)^{\frac{z_1 - z_2}{z_1 - z_2}} = \left(\frac{1 - X_{A1}}{1 - X_{A2}} \right)^{\frac{z_1 - z_2}{z_1 - z_2}}$$

What is the rate of Evaporation?

Answer: $N_{A,z}$

$\Rightarrow C_1$

$X_{A1} = \frac{P^*}{P} = 0.0728744$ (see tables for $P^*(H_2O, T)$)

$X_{A2} = 0.02$ (given)

$c = \frac{\rho}{M} = \frac{P}{RT} = 3.891367 \times 10^{-5} \frac{\text{mol}}{\text{cm}^3}$

$P D_{AB} = 2.674 \frac{\text{m}^2 \text{Pa}}{\text{s}}$ (App J)

... ANSWER:

Then, we answered the question:

$$N_{A,z} = C_1 = \frac{cD_{AB}}{(z_1 - z_2)} \ln \left(\frac{1 - X_{A1}}{1 - X_{A2}} \right)$$

The rate of evaporation
 $A_{xs} N_{A,z} = 3.9 \times 10^{-6} \text{ mol/s.}$

$$A_{xs} = \frac{\pi D_{\text{tank}}^2}{4}$$

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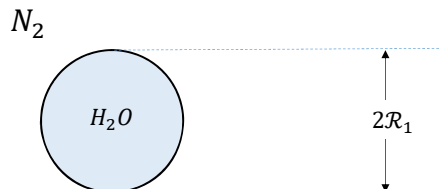
The primary goals are

QUICK START

- to grow our ability to troubleshoot engineering problems
- To explore "classic" mass transfer circumstances and add them to our tool belt

Let's do another problem

Example 2: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). What is the rate of evaporation and how does the water concentration vary in the gas?



Ver 1

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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). What is the rate of evaporation and how does the water concentration vary in the gas?

Let's Interrogate the problem.

Ver 1

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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). What is the rate of evaporation and how does the water concentration vary in the gas?

Why does the water evaporate?

What limits the rate of evaporation?

What could be done to accelerate the evaporation?

What could be done to slow down the evaporation?

What is the driving physics?

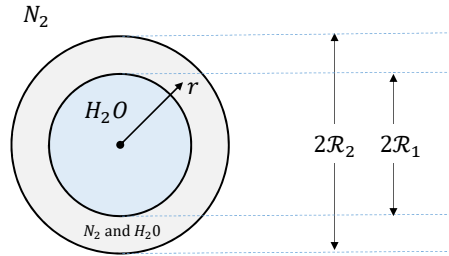
Can we use any ideas from previous experience?

Ver 1

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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.



We are developing a model to address the questions of interest

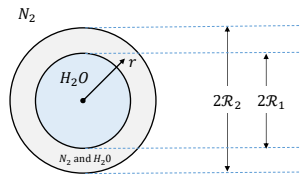
Ver 2

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13
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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 as a function distance from the droplet? You may assume ideal gas properties for air.



Ver 2

SOLVE

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QUICK START

SOLUTION:

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

See hand slides

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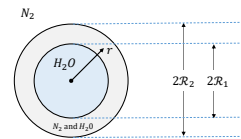
QUICK START

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.

Assumptions:

- Steady diffusion; stagnant air
- **Uniform film** surrounds droplet
- Ideal gas
- Constant temperature and pressure
- Constant c, D_{AB}



Solution:

$x_A(r)$

$$\frac{1 - x_{A1}}{1 - x_{A2}} = \left(\frac{1 - x_{A2}}{1 - x_{A1}} \right) \left(\frac{\frac{1}{R_1} - \frac{1}{r}}{\frac{1}{R_1} - \frac{1}{R_2}} \right)$$

Homework problem 3.14 do algebra; problem 3.8 plot this solution

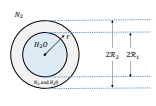
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QUICK START

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

↩

We can now explore these assumptions, and modify, if needed, for more complex problems.

Solution:

$x_A(r)$

$$\frac{1 - x_A}{1 - x_{A1}} = \left(\frac{1 - x_{A2}}{1 - x_{A1}} \right) \left(\frac{\frac{1}{R_1} \frac{1}{r}}{\frac{1}{R_1} \frac{1}{R_2}} \right)$$

Let's Interrogate the problem.

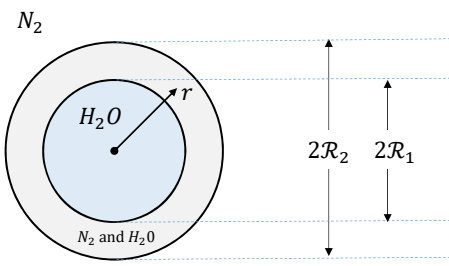
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QUICK START

Film model of mass transfer

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.



Assumptions:

- Uniform film
- Ideal gas
- Constant pressure
- Constant temperature

How good are these assumptions?

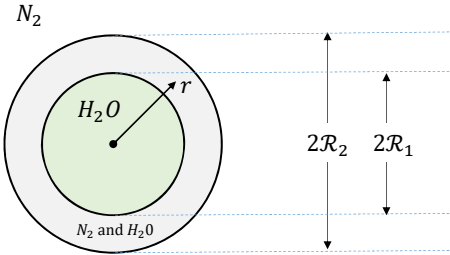
Are there energy issues?

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Film model of mass transfer (more complex) 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. We can model the diffusion process as shown in the figure. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet?

Note: *not* isothermal



$\Delta \hat{h}_{\text{vap}} \neq 0$

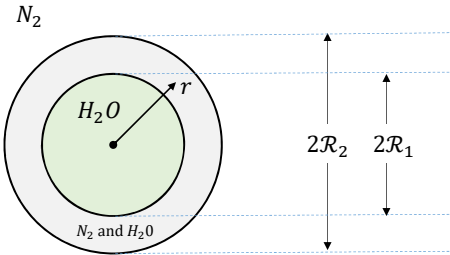
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Film model of mass transfer (more complex) QUICK START

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Note: *not* isothermal



$\Delta \hat{h}_{\text{vap}} \neq 0$

What does changing temperature impact?

How do we modify the model?

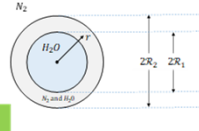
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Film model of mass transfer (more complex)

Where did we assume "isothermal" in our previous solution?

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.



The Film Model of mass transfer

Ver 2

Equation of Species Mass Balance in Terms of Φ

Quantities - Φ is a scalar, and \mathbf{N}_A is a vector. \mathbf{N}_A is the species mass flux vector, and Φ is the species mass flux scalar.

Species mass balance: $\nabla \cdot \mathbf{N}_A = \dot{S}_A$

Species mass flux: $\mathbf{N}_A = -D_{AB} \nabla x_A + x_A \mathbf{N}$

Species mass flux scalar: $\Phi_A = -D_{AB} \frac{dx_A}{dr} + x_A N_r$

Species mass flux vector: $\mathbf{N}_A = -D_{AB} \nabla x_A + x_A \mathbf{N}$

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Microscopic species A mass bal³

- steady
- no rxn
- Φ symmetry (see p2)

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

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

$$r^2 N_{Ar} = \Phi = C_1$$

$$N_{Ar} = \frac{C_1}{r^2}$$

Fick's Law of Diffusion

- constant T
- Φ symmetric
- Φ symmetric
- $N_{Ar} = x_A N_r = -c D_{AB} \frac{dx_A}{dr}$ (assume const)

$$c = \frac{n}{V} = \frac{P}{RT} = \text{const}$$

Solve

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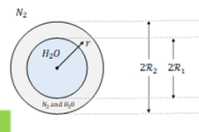
21

Film model of mass transfer (more complex)

Where did we assume "isothermal" in our previous solution?

When we integrated to obtain $x_A(r)$.

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.



The Film Model of mass transfer

Ver 2

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Microscopic species A mass bal³

- steady
- no rxn
- Φ symmetry (see p2)

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

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

$$r^2 N_{Ar} = \Phi = C_1$$

$$N_{Ar} = \frac{C_1}{r^2}$$

Fick's Law of Diffusion

- constant T
- Φ symmetric
- Φ symmetric
- $N_{Ar} = x_A N_r = -c D_{AB} \frac{dx_A}{dr}$ (assume const)

$$c = \frac{n}{V} = \frac{P}{RT} = \text{const}$$

Solve

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22

Film model of mass transfer (more complex) 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. We can model the diffusion process as shown in the figure. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$. 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; you may assume that the diffusivity varies with temperature as follows:

$$D_{AB}(T)/D_{AB,1} = (T/T_1)^{3/2}$$

N_2

H_2O

$N_2 \text{ and } H_2O$

r

$2\mathcal{R}_2$ $2\mathcal{R}_1$

Note: not isothermal

HW 3.7 (stretch)

Ver 4

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Film model of mass transfer (more complex) QUICK START

Ver 4

Assumptions:

- Uniform film surrounds droplet
- Ideal gas
- Temperature follows power law
- Diffusivity follows power law
- Pressure is constant

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. We can model the diffusion process as shown in the figure. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$. What is the water mole fraction in the film as a function of radial position? You may assume ideal gas properties for air; you may assume that the diffusivity varies with temperature as follows:

$$D_{AB}(T)/D_{AB,1} = (T/T_1)^{3/2}$$

N_2

H_2O

$N_2 \text{ and } H_2O$

r

$2\mathcal{R}_2$ $2\mathcal{R}_1$

Note: not isothermal

Solution:

$x_A(r)$

$$\frac{1 - x_{A1}}{1 - x_{A2}} = \left(\frac{1 - x_{A2}}{1 - x_{A1}} \right) \left(\frac{\frac{1}{\mathcal{R}_1^{1+n/2}} \frac{1}{r^{1+n/2}}}{\frac{1}{\mathcal{R}_1^{1+n/2}} \frac{1}{\mathcal{R}_2^{1+n/2}}} \right)$$

HW 3.7

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Introduction to Diffusion and Mass Transfer in Mixtures QUICK START

Recurring Modeling Assumptions in Diffusion (“Classics”)

- Near a liquid-gas interface, the region in the gas near the liquid is a film where slow diffusion takes place
- The vapor near the liquid-gas interface is often saturated (Raoult’s law, $x_A = p_A^*/p$)
- If component A has no sink, flux $N_A = 0$.
- If A diffuses through stagnant B , $N_B = 0$.
- If A is dilute in B , we can neglect the convection term ($N_{Az} = J_{Az}^*$)
- Because diffusion is slow, we can make a quasi-steady-state assumption
-
-
-
-
-
-

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We have been performing a “Quick Start,”

And have found the combined molar flux formulation useful.

It turns out that there are many interesting and applicable problems we can address readily with this form of the species mass balance.

Microscopic species A mass balance—Five forms	
In terms of mass flux and mass concentrations	$\rho \left(\frac{\partial \omega_A}{\partial t} + \mathbf{v} \cdot \nabla \omega_A \right) = -\nabla \cdot \mathbf{J}_A + r_A$ $= \rho D_{AB} \nabla^2 \omega_A + r_A$
In terms of molar flux and molar concentrations	$c \left(\frac{\partial x_A}{\partial t} + \mathbf{v} \cdot \nabla x_A \right) = -\nabla \cdot \mathbf{J}_A + R_A$ $= c D_{AB} \nabla^2 x_A$
In terms of combined molar flux and molar concentrations	$\frac{dc_A}{dt} = -\nabla \cdot \mathbf{N}_A + R_A$

Let’s jump in!

We’ll do a “Quick Start” and get into some examples and return to the “why” of it all a bit later.

Microscopic species mass balance in terms of combined molar flux N_A


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There are times it is not useful. We need to go back and discuss *how/why/when* this all works.


Various forms of Fick's Law (and the species mass balances that employ them)

<p>Mass flux</p> $j_A = -\rho D_{AB} \nabla \omega_A$	<p>Molar flux</p> $J_A = -c D_{AB} \nabla x_A$	<p>Combined molar flux</p> $N_A = x_A(N_A + N_B) - c D_{AB} \nabla x_A$
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FRONT







pages.mtu.edu/~fmorriso/cm3120/Homeworks_Readings.html
50
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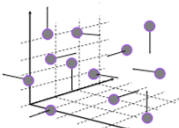
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Now, Cycling Back:

Diffusion and Mass Transfer

CM3120 Transport/Unit Operations 2

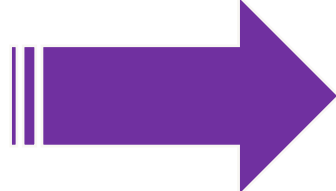
Diffusion and Mass Transfer





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