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

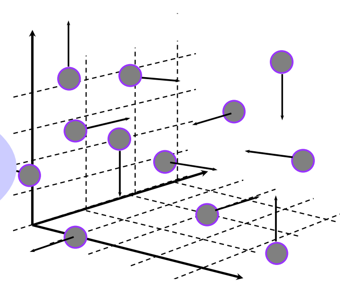
1

CM3120: Module 3

Module 3 Lecture IV

Fick's Law of Diffusion

(Cycling back)



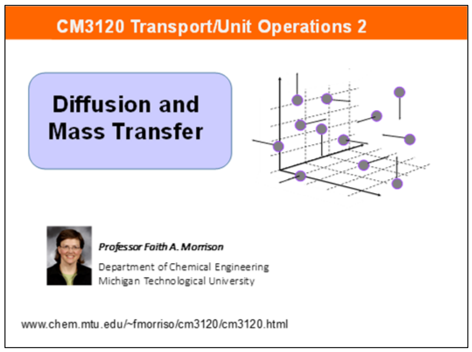
Professor Faith A. Morrison
Department of Chemical Engineering
Michigan Technological University

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

2

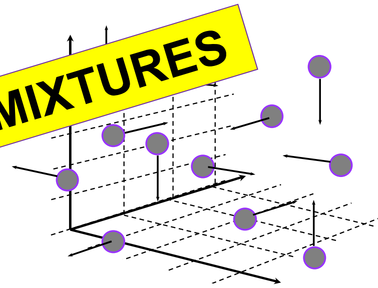
Now, Cycling Back:

Diffusion and Mass Transfer



CM3120 Transport/Unit Operations 2

Diffusion and Mass Transfer ^ **in MIXTURES**

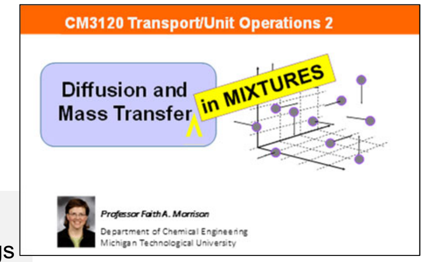


Professor Faith A. Morrison
Department of Chemical Engineering
Michigan Technological University

We began a few weeks ago…

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

We first introduced the topic of diffusion and mass transfer a few weeks ago…



Summary:

- Occurs in mixtures; this complicates things
- Is *slow* and often the rate-limiting process
- Mass is conserved, but often moles are more convenient to keep track of what's going on
- Is the third transport field (momentum, energy, species A mass)
- Up to mass transfer, have been readily modeling using the *continuum*; this approach needs to be adapted to mixtures
- We had decided to "skip ahead" **(QUICK START)** to avoid getting bogged down…

Species A transport law:
Fick's law of diffusion

$$j_{A,z} = -\rho D_{AB} \frac{\partial \omega_A}{\partial z}$$

A diffuses in B

Recap:

QUICK START

Species Fluxes

The community has found use for four (actually more) different fluxes. The differences in the various fluxes are related to several questions:

Flux of what? And due to what mechanism?

$\underline{N}_A$ – combined molar flux (includes both convection and diffusion)
$\underline{n}_A$ – combined mass flux (includes both convection and diffusion)
$\underline{j}_A$ – mass flux (diffusion only)
$\underline{J}_A^*$ – molar flux (diffusion only)

Microscopic species A mass balance

$$\rho\left(\frac{\partial \omega_A}{\partial t} + \underline{v}\cdot\nabla\omega_A\right) = \rho D_{AB}\nabla^2\omega_A + r_A$$

rate of change; convection; diffusion (all directions); source (mass of species A generated by homogeneous reaction per time)

Written relative to what velocity?

$\underline{N}_A$ – relative to stationary coordinates
$\underline{n}_A$ –relative to stationary coordinates
$\underline{j}_A$ – relative to the mass average velocity $\underline{v}$
$\underline{J}_A^*$ – relative to the molar average velocity $\underline{v}^*$

These different definitions lead to different forms for the **microscopic species mass** balance and for **the transport law**.

These different fluxes are a significant complication. → It will take some time and practice to get used to all this →

QUICK START

Recap:

Microscopic species A mass balance—Five forms

In terms of mass flux and mass concentrations	$\rho\left(\frac{\partial \omega_A}{\partial t} + \underline{v}\cdot\nabla\omega_A\right) = -\nabla\cdot\underline{j}_A + r_A$ $= \rho D_{AB}\nabla^2\omega_A + r_A$
In terms of molar flux and molar concentrations	$c\left(\frac{\partial x_A}{\partial t} + \underline{v}^*\cdot\nabla x_A\right) = -\nabla\cdot\underline{J}_A^* + (x_B R_A - x_A R_B)$ $= c D_{AB}\nabla^2 x_A + (x_B R_A - x_A R_B)$
In terms of combined molar flux and molar concentrations	$\frac{\partial c_A}{\partial t} = -\nabla\cdot\underline{N}_A + R_A$

These different definitions lead to **different forms** for the **microscopic species mass balance** and for the **species transport law**, Fick's law.

It will take some time and practice to get used to all this

QUICK START

Recap:

Various quantities in diffusion and mass transfer

How much is present: $c x_A = c_A = \frac{1}{M_A}(\rho_A) = \frac{1}{M_A}(\rho\omega_A)$

$\underline{j}_A \equiv$ **mass** flux of species A relative to a mixture's **mass average velocity**, $\underline{v}$
$= \rho_A(\underline{v}_A - \underline{v})$
$\underline{j}_A + \underline{j}_B = 0$, i.e. these fluxes are measured relative to the mixture's center of mass

$\underline{n}_A \equiv \rho_A\underline{v}_A = \underline{j}_A + \rho_A\underline{v} =$ **combined mass** flux relative to **stationary coordinates**
$\underline{n}_A + \underline{n}_B = \rho\underline{v}$

$\underline{J}_A^* \equiv$ **molar** flux relative to a mixture's **molar average velocity**, $\underline{v}^*$
$= c_A(\underline{v}_A - \underline{v}^*)$
$\underline{J}_A^* + \underline{J}_B^* = 0$

$\underline{N}_A \equiv c_A\underline{v}_A = \underline{J}_A^* + c_A\underline{v}^* =$ **combined molar** flux relative to **stationary coordinates**
$\underline{N}_A + \underline{N}_B = c\underline{v}^*$

$\underline{v}_A \equiv$ velocity of species A in a mixture, i.e. average velocity of all molecules of species A within a small volume
$\underline{v} = \omega_A\underline{v}_A + \omega_B\underline{v}_B \equiv$ mass average velocity; same velocity as in the microscopic momentum and energy balances
$\underline{v}^* = x_A\underline{v}_A + x_B\underline{v}_B \equiv$ molar average velocity

Part of the problem is that we have grown comfortable with the *continuum*, but now we are peering into the details of the continuum

It will take some time and practice to get used to all this

Recap:

QUICK START

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

Mass flux	Molar flux	Combined molar flux
$\underline{j}_A = -\rho D_{AB} \nabla \omega_A$	$\underline{J}_A^* = -c D_{AB} \nabla x_A$	$\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - c D_{AB} \nabla x_A$

FRONT

pages.mtu.edu/~fmorriso/cm3120/Homeworks_Readings.html

We will be introduced to handy worksheets and to the common assumptions and boundary conditions (just like in momentum and energy balances) → It will take some time and practice to get used to all this →

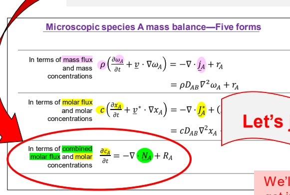
QUICK START

We skipped to one version of the *Species A mass balance* (and Fick's law) and got some practice.

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

$$\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - c D_{AB} \nabla x_A$$

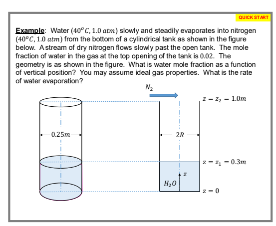
It turns out that there are many interesting and applicable problems we can address readily with **this** form of the species mass balance.



Let's jump in!

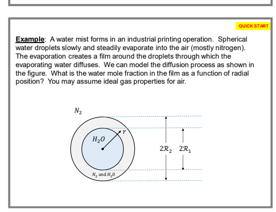
Microscopic species mass balance in terms of combined molar flux $\underline{N}_A$

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



QUICK START

Example: Water $(40^o C, 1.0\ atm)$ slowly and steadily evaporates into nitrogen $(40^o C, 1.0\ atm)$ 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. The geometry is as shown in the figure. What is water mole fraction as a function of vertical position? You may assume ideal gas properties. What is the rate of water evaporation?



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. We can model the diffusion process as shown in the figure. What is the water mole fraction in the film as a function of radial position? You may assume ideal gas properties for air.

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 $\underline{N}_A = 0$.
- If A diffuses through stagnant B, $\underline{N}_B = 0$.
- 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
-
-
-
-
-
-

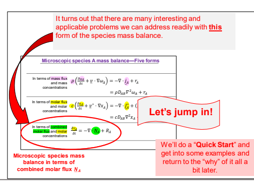
11

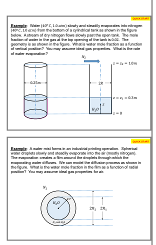
QUICK START

We skipped to one version of the *Species A mass balance* (and Fick's law) and got some practice.

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

$$\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$$





The **QUICK START** has perhaps led to the impression that the ***combined molar flux*** version is all we need to address problems in mass transfer…

This is unfortunately ***not true***. We have thus far been selective in choosing problems addressable by that approach.

To succeed more broadly, we need to address additional complexities of mixtures and mass transfer.

12

Introduction to Diffusion and Mass Transfer in Mixtures

Questions we skipped:

Where does Fick's law come from?

Why so many definitions of flux?

Will this approach (combined molar flux) work for all circumstances?

Species Fluxes

The community has found use for four (actually more) different fluxes. The differences in the various fluxes are related to several questions:

Flux of what? And due to what mechanism?

- $\underline{N}_A$ – combined molar flux (includes convection and diffusion)
- $\underline{n}_A$ – combined mass flux (includes convection and diffusion)
- $\underline{j}_A$ – mass flux (diffusion only)
- $\underline{J}_A^*$ – molar flux (diffusion only)

Microscopic species A mass balance

$$\rho\left(\frac{\partial \omega_A}{\partial t} + \underline{v}\cdot\nabla\omega_A\right) = \rho D_{AB}\nabla^2\omega_A + r_A$$

rate of change; convection; diffusion (all directions); source (mass of species A generated by homogeneous reaction per time)

Written relative to what velocity?

- $\underline{N}_A$ – relative to stationary coordinates
- $\underline{n}_A$ – relative to stationary coordinates
- $\underline{j}_A$ – relative to the mass average velocity $\underline{v}$
- $\underline{J}_A^*$ – relative to the molar average velocity $\underline{v}^*$

These different definitions lead to different forms for the **microscopic species mass** balance and for **the transport law**.

13

Introduction to Diffusion and Mass Transfer in Mixtures

Questions we skipped:

Where does Fick's law come from?

Why so many definitions of flux?

Will this approach (combined molar flux) work for all circumstances?

Species Fluxes

The community has found use for four (actually more) different fluxes. The differences in the various fluxes are related to several questions:

Flux of what? And due to what mechanism?

- $\underline{N}_A$ – combined molar flux (includes convection and diffusion)
- $\underline{n}_A$ – combined mass flux (includes convection and diffusion)
- $\underline{j}_A$ – mass flux (diffusion only)
- $\underline{J}_A^*$ – molar flux (diffusion only)

Microscopic species A mass balance

$$\rho\left(\frac{\partial \omega_A}{\partial t} + \underline{v}\cdot\nabla\omega_A\right) = \rho D_{AB}\nabla^2\omega_A + r_A$$

rate of change; convection; diffusion (all directions); source (mass of species A generated by homogeneous reaction per time)

Written relative to what velocity?

- $\underline{N}_A$ – relative to stationary coordinates
- $\underline{n}_A$ – relative to stationary coordinates
- $\underline{j}_A$ – relative to the mass average velocity $\underline{v}$
- $\underline{J}_A^*$ – relative to the molar average velocity $\underline{v}^*$

These different definitions lead to different forms for the **microscopic species mass** balance and for **the transport law**.

We cycle back now to return to this discussion

14

Transport Laws, momentum and heat:

Part I: Momentum Transfer

Momentum transfer:

$$\tilde{\tau}_{21} = \mu\left(\frac{dv_1}{dx_2}\right)$$

momentum flux ($\tilde{\tau}_{21}$); viscosity (μ); velocity gradient ($\frac{dv_1}{dx_2}$)

Newton's law of viscosity

Part II: Heat Transfer

Heat transfer:

$$\frac{q_x}{A} = -k\frac{dT}{dx}$$

heat flux ($\frac{q_x}{A}$); thermal conductivity (k); temperature gradient ($\frac{dT}{dx}$)

Fourier's law of heat conduction

15

Part I: Momentum Transfer

Momentum transfer:

$$\tau_{21} = (-\tilde{\tau}_{21}) = -\mu\left(\frac{dv_1}{dx_2}\right)$$

momentum flux; viscosity; velocity gradient

Newton's law of viscosity

Part II: Heat Transfer

Heat transfer:

$$\frac{q_x}{A} = -k\frac{dT}{dx}$$

heat flux; thermal conductivity; temperature gradient

Fourier's law of conduction

Now:

Part III: Mass Transfer

Mass transfer:

$$j_{A,x} = -\rho D_{AB}\frac{\partial \omega_A}{\partial x}$$

Mass flux of species A ($j_{A,x}$); diffusivity (D_{AB}); species mass fraction gradient ($\frac{\partial \omega_A}{\partial x}$)

Fick's law of diffusion

16

Part I: Momentum Transfer

Momentum transfer: (viscosity)

$$\tau_{21} = (-\tilde{\tau}_{21}) = -\mu\left(\frac{dv_1}{dx_2}\right)$$

momentum flux; velocity gradient

Newton's law of viscosity

Part II: Heat Transfer

Heat transfer: (thermal conductivity)

q_x ... dT ... radient

Fourier's law of conduction

Now:

Part III: Mas

Mass transf ... fusivity

$$j_{A,x} = -\rho D_{AB} \frac{\quad}{\partial x}$$

Mass flux of species A; species mass fraction gradient

Fick's law of diffusion

Where do these equations come from?

 17

The Physics of the Transport Laws

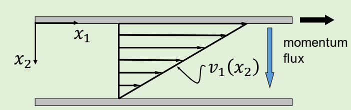
Part I: Momentum Transfer

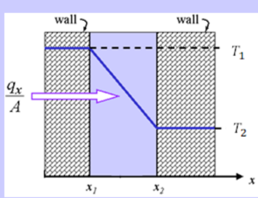
Momentum transfer: (viscosity)

$$\tau_{21} = (-\tilde{\tau}_{21}) = -\mu\left(\frac{dv_1}{dx_2}\right)$$

momentum flux; velocity gradient

Newton's law of viscosity





Part II: Heat Transfer

Heat transfer: (thermal conductivity)

$$\frac{q_x}{A} = -k\frac{dT}{dx}$$

heat flux; temperature gradient

Fourier's law of conduction

Part III: Mass Transfer

Mass transfer: (diffusivity)

$$j_{A,x} = -\rho D_{AB}\frac{\partial \omega_A}{\partial x}$$

Mass flux of species A; species mass fraction gradient

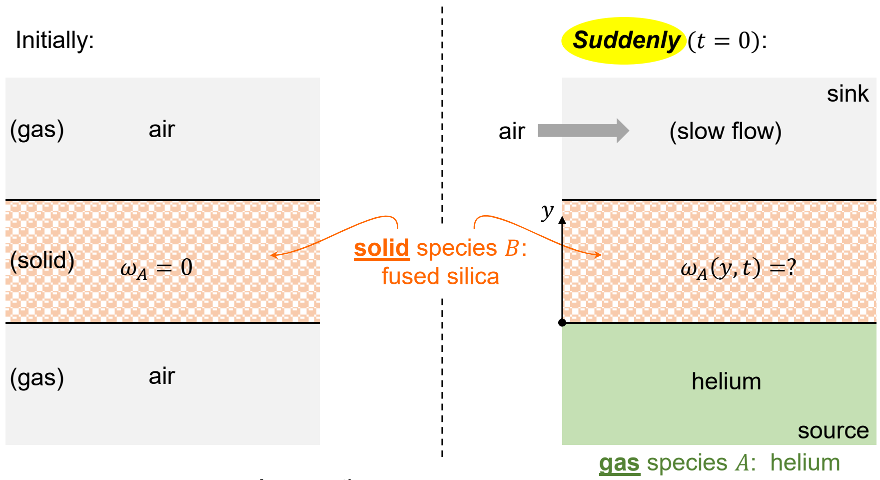
Fick's law of diffusion

Where does *this* equation come from?

 18

Simple One-dimensional Species Mass Diffusion

What is the physics behind the mass diffusion transport law?



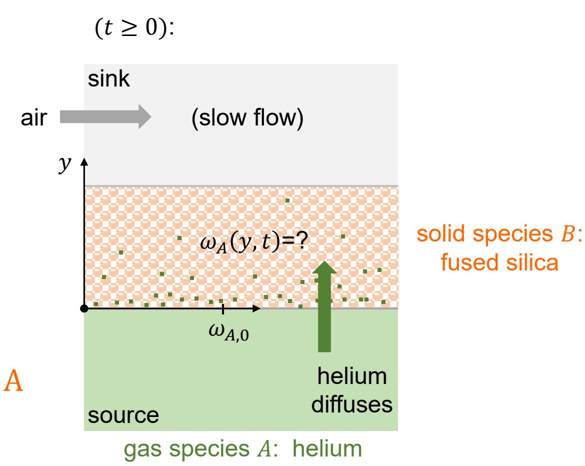
Assumptions:
- wide, deep⇒ 1D diffusion
- no reaction
- species B not moving

BSL2, p514

Simple One-dimensional Species Mass Diffusion

What does $\omega_A(y,t)$ look like?

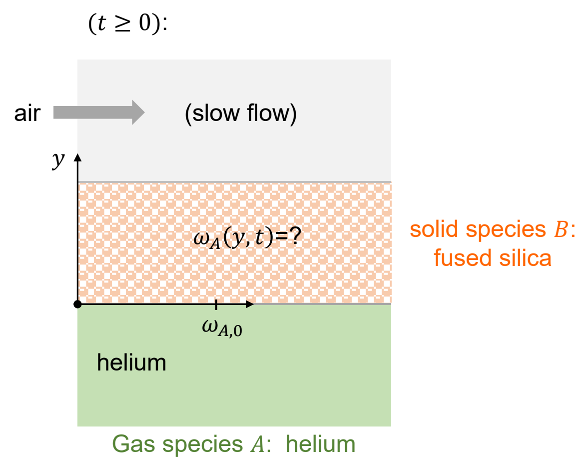
ω_A = mass fraction of A



BSL2, p514

Simple One-dimensional Species Mass Diffusion

What does $\omega_A(y,t)$ look like?

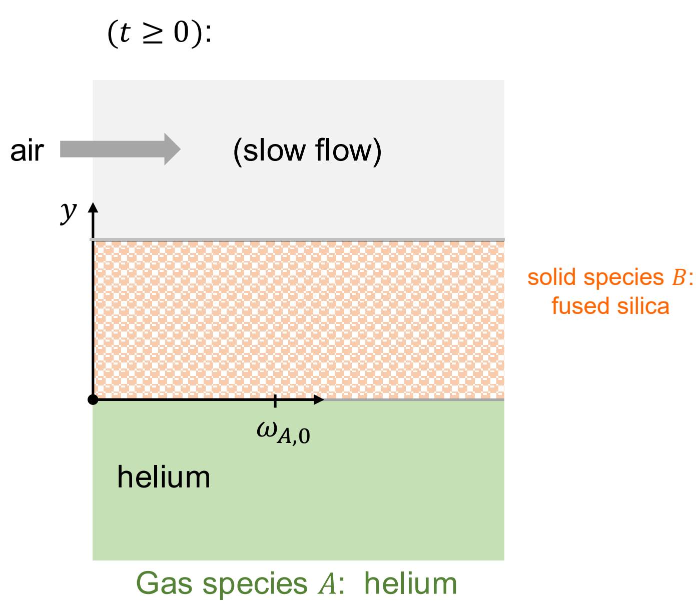


You try.

BSL2, p514

Simple One-dimensional Species Mass Diffusion

- $\omega_A(y,t)$=?
- What is the domain we're asking about?

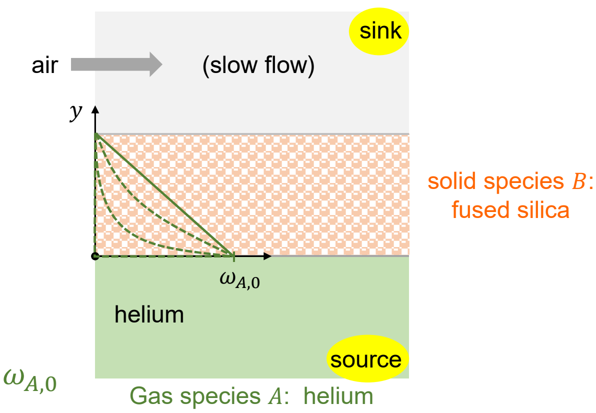


BSL2, p514

Simple One-dimensional Species Mass Diffusion

Suddenly $(t = 0)$:

What does $\omega_A(y,t)$ look like?



At steady state,

$$\omega_A(y,t) = -\frac{\omega_{A,0}}{D}y + \omega_{A,0}$$

BSL2, p514

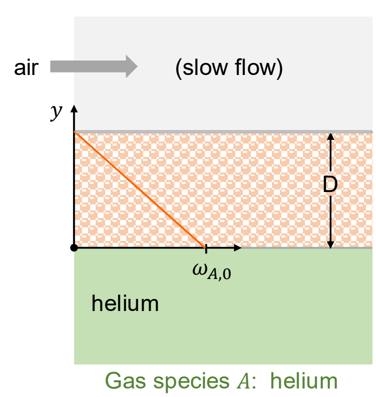
 23

Simple One-dimensional Species Mass Diffusion

Suddenly $(t = 0)$:

At steady state,

$$\omega_A(y,t) = -\frac{\omega_{A,0}}{D}y + \omega_{A,0}$$



$$\text{mass flux} = \rho D_{AB}\left(\frac{0-\omega_{A,0}}{y_2 - y_1}\right)$$

$$j_{A,y} = -\rho D_{AB}\frac{d\omega_A}{dy}$$

Fick's law of diffusion

(in terms of <u>mass</u> flux)

D_{AB} = Diffusion coefficient of A through B

$j_{A,y}$ = **mass** flux of A through B
$[=] \frac{kg\ A}{m^2 s}$

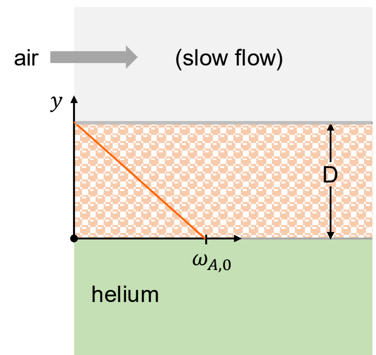
BSL2, p514

 24

Simple One-dimensional Species Mass Diffusion

This is the fundamental version of Fick's Law (1D)

Suddenly $(t = 0)$:



Gas species A: helium

$$j_{A,y} = -\rho D_{AB} \frac{d\omega_A}{dy}$$

Fick's law of diffusion

(in terms of *mass* *flux)*

D_{AB} = Diffusion coefficient of A through B

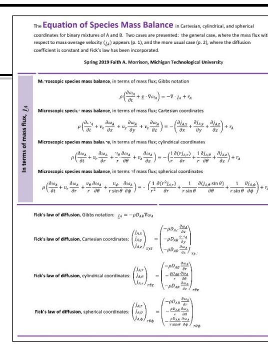
$j_{A,y}$ = **mass** flux of A through B

$[=] \frac{kg\ A}{m^2 s}$

BSL2, p514

 25

Law of Species Diffusion



This is the fundamental version of Fick's Law (3D)

Gibbs notation: $\underline{j}_A = -\rho \mathrm{D}_{\mathrm{AB}} \nabla \omega_A$

Fick's law of diffusion

$$\underline{j}_A = \begin{pmatrix} -\rho \mathrm{D}_{\mathrm{AB}} \frac{\partial \omega_A}{\partial x} \\ -\rho \mathrm{D}_{\mathrm{AB}} \frac{\partial \omega_A}{\partial y} \\ -\rho \mathrm{D}_{\mathrm{AB}} \frac{\partial \omega_A}{\partial z} \end{pmatrix}_{xyz}$$

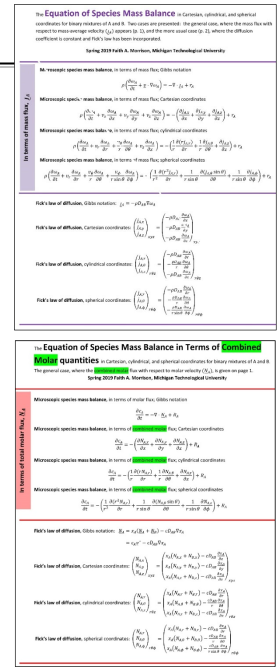
- Mass diffuses flows **down** a concentration gradient
- Flux is proportional to magnitude of concentration gradient

 26

Law of Species Diffusion

This is the fundamental version of Fick's Law (3D)

But it is *not* the one we have been using!


The Equation of Species Mass Balance in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. Two cases are presented: the general case, where the mass flux with respect to mass-average velocity (j_A) appears (p. 1), and the more usual case (p. 2), where the diffusion coefficient is constant and Fick's law has been incorporated.

Spring 2019 Faith A. Morrison, Michigan Technological University

In terms of mass flux, j_A

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

$$\rho\left(\frac{\partial \omega_A}{\partial t}+\underline{v}\cdot\nabla\omega_A\right)=-\nabla\cdot \underline{j}_A+r_A$$

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

$$\rho\left(\frac{\partial \omega_A}{\partial t}+v_x\frac{\partial \omega_A}{\partial x}+v_y\frac{\partial \omega_A}{\partial y}+v_z\frac{\partial \omega_A}{\partial z}\right)=-\left(\frac{\partial j_{A,x}}{\partial x}+\frac{\partial j_{A,y}}{\partial y}+\frac{\partial j_{A,z}}{\partial z}\right)+r_A$$

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

$$\rho\left(\frac{\partial \omega_A}{\partial t}+v_r\frac{\partial \omega_A}{\partial r}+\frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta}+v_z\frac{\partial \omega_A}{\partial z}\right)=-\left(\frac{1}{r}\frac{\partial (r j_{A,r})}{\partial r}+\frac{1}{r}\frac{\partial j_{A,\theta}}{\partial \theta}+\frac{\partial j_{A,z}}{\partial z}\right)+r_A$$

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

Fick's law of diffusion, Gibbs notation: $\underline{j}_A=-\rho D_{AB}\nabla\omega_A$

Fick's law of diffusion, Cartesian coordinates

Fick's law of diffusion, cylindrical coordinates:

$$\begin{pmatrix} j_{A,r}\\ j_{A,\theta}\\ j_{A,z}\end{pmatrix}_{r\theta z}=\begin{pmatrix}-\rho D_{AB}\frac{\partial\omega_A}{\partial r}\\ -\frac{\rho D_{AB}}{r}\frac{\partial\omega_A}{\partial\theta}\\ -\rho D_{AB}\frac{\partial\omega_A}{\partial z}\end{pmatrix}_{r\theta z}$$

Fick's law of diffusion, spherical coordinates:

$$\begin{pmatrix} j_{A,r}\\ j_{A,\theta}\\ j_{A,\phi}\end{pmatrix}_{r\theta\phi}=\begin{pmatrix}-\rho D_{AB}\frac{\partial\omega_A}{\partial r}\\ -\frac{\rho D_{AB}}{r}\frac{\partial\omega_A}{\partial\theta}\\ -\frac{\rho D_{AB}}{r\sin\theta}\frac{\partial\omega_A}{\partial\phi}\end{pmatrix}_{r\theta\phi}$$

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

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

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

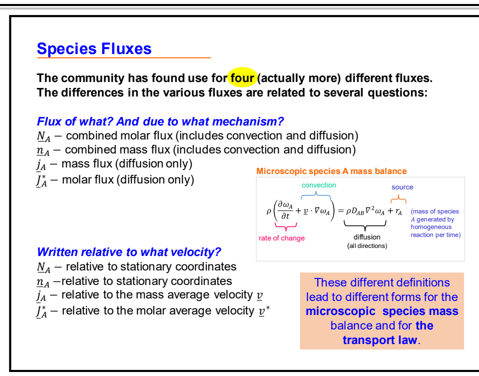
Fick's law of diffusion, Gibbs notation

Fick's law of diffusion, Cartesian coordinates

Fick's law of diffusion, cylindrical coordinates

Fick's law of diffusion, spherical coordinates

Law of Species Diffusion



***QUESTION*:**

Why so many versions of species A flux?

***Answer*:**

"Breaking into" the continuum view to analyze the motion of individual species in a mixture complicates the situation. There are several options, and none is perfect for all situations.

Let's take a look

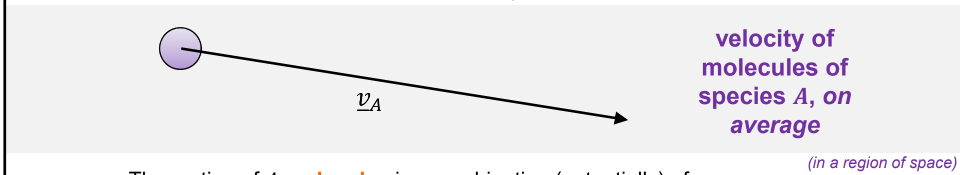
Describing Binary Diffusion

A mixture of two species: *What goes where and why*

- There are many molecules of species A in some region of interest
- In the region of interest, $\underline{v}_A$ is the **average velocity** (speed and direction) of the A molecules:

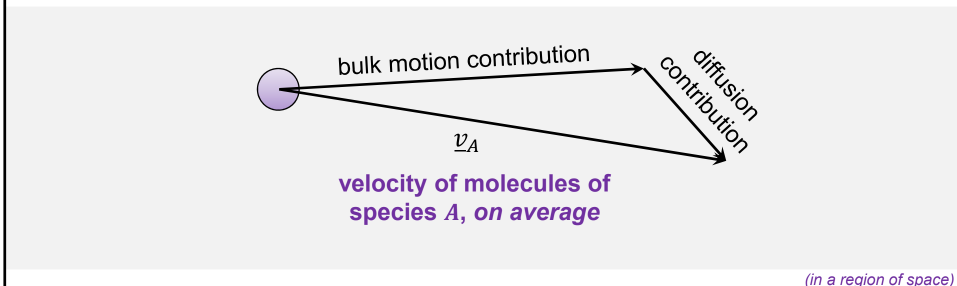
$$\underline{v}_A = \frac{1}{n_T}\sum_{i=1}^{n_T} \underline{v}_{A,i}$$

(a regular average)



- The motion of A **molecules** is a combination (potentially) of
  - **bulk motion**—this is the motion caused by driving pressure gradients, by moving boundaries, by all the causes studied for homogeneous materials when we studied momentum conservation with the continuum approach
  - **Diffusion**—this motion is caused by concentration gradients.
  - **These two motions need not be collinear**

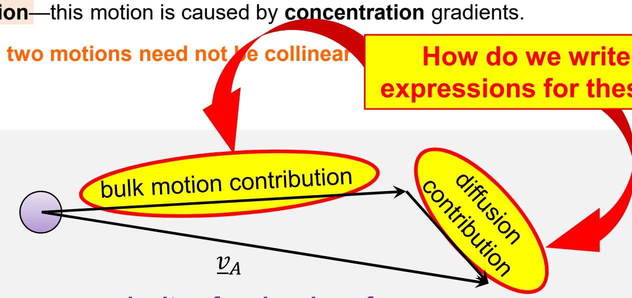
- The motion of A **molecules** is a combination (potentially) of
  - **bulk motion** of the mixture—this is the motion caused by driving pressure gradients, by moving boundaries, by all the causes studied for **homogeneous** materials when we studied momentum conservation
  - **diffusion**—this motion is caused by **concentration** gradients.
  - **These two motions need not be collinear**



“Flux” of Species A in a Mixture with Species B

- The motion of A **molecules** is a combination (potentially) of
  - **bulk motion** of the mixture—this is the motion caused by driving pressure gradients, by moving boundaries, by all the causes studied for **homogeneous** materials when we studied momentum conservation
  - **diffusion**—this motion is caused by **concentration** gradients.
  - **These two motions need not be collinear**

How do we write expressions for these?



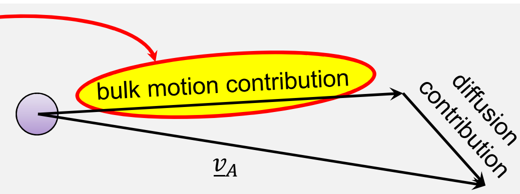
velocity of molecules of species A, *on average*

(in a region of space)

 31

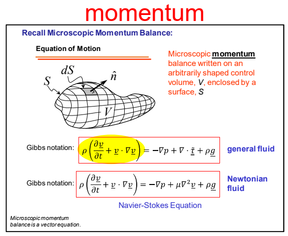
“Flux” of Species A in a Mixture with Species B

Is this $\underline{v}$?

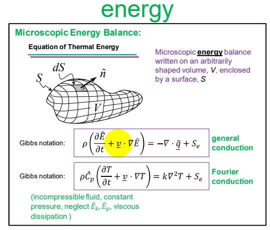


We’ve already defined $\underline{v}$ and used it when we studied momentum and heat transport in homogeneous materials using the continuum model.

momentum



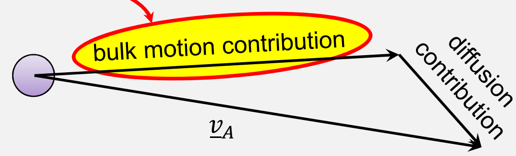
energy



 32

"Flux" of Species A in a Mixture with Species B

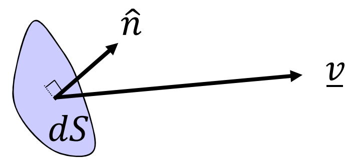
Is this $\underline{v}$?



In transport (*of momentum and energy*) in homogeneous phases (not mixtures):

local mass flow

$$\rho\, d\dot{V} = \rho(\hat{n} \cdot \underline{v})\, dS$$



What does this mean when applied to a mixture of A and B?

 33

"Flux" of Species A in a Mixture with Species B

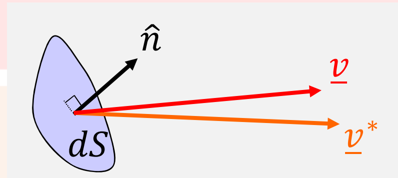
When we apply the other transport laws to mixtures of A and B, **they work**, if $\underline{v}$ is the **mass** average velocity of the **molecular** velocities $\underline{v}_A$ and $\underline{v}_B$

local mass flow

mass average velocity of individual molecules

(continuum is divided into mass "particles")

$$\rho\, d\dot{V} = \rho(\hat{n} \cdot \underline{v})\, dS$$



If, however, the **molar** average velocity $\underline{v}^*$ of the molecules in a mixture is calculated, a local molar flow is readily obtained and ***it is not the same as $\underline{v}$:***

local molar flow

(continuum is divided into molar "particles")

$$c\, d\dot{V} = c(\hat{n} \cdot \underline{v}^*)\, dS$$

molar average velocity of individual molecules

Sorry about the re-used nomenclature: $\underline{v}^*$ = the molar average velocity

 34

"Flux" of Species A in a Mixture with Species B

When we apply the other transport laws to mixtures of A and B, **they work**, if $\underline{v}$ is the **mass** average velocity of the **molecular** velocities $\underline{v}_A$ and $\underline{v}_B$

local mass flow — *mass* average velocity of individual molecules

$$\underline{v} = \omega_A \underline{v}_A + \omega_B \underline{v}_B$$

$$\rho\, d\dot{V} = \rho(\,\hat{n}\cdot\underline{v})\, dS$$

This is what I mean when I say we are **"breaking into"** the continuum picture.

If, however, the **molar** average velocity $\underline{v}^*$ of the molecules in a mixture is calculated, a local molar flow is readily obtained and ***it is not the same as*** $\underline{v}$:

local molar flow

$$c\, d\dot{V} = c(\,\hat{n}\cdot\underline{v}^*)\, dS$$

molar average velocity of individual molecules

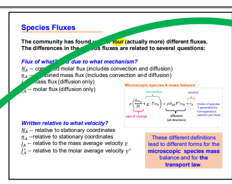
$$\underline{v}^* = x_A \underline{v}_A + x_B \underline{v}_B$$

Sorry about the re-used nomenclature: v^* = the molar average velocity

 35

Law of Species Diffusion

QUESTION: Why so many versions of species A flux?



Answer: "Breaking into" the continuum view to analyze the motion of individual species in a mixture complicates the situation. There are several options, and none is perfect.

This is what I mean when I say we are ***"breaking into"*** the continuum picture.

"Flux" of Species A in a Mixture with Species B

When we apply the other transport laws to mixtures of A and B, **they work**, if $\underline{v}$ is the **mass** average velocity of the **molecular** velocities $\underline{v}_A$ and $\underline{v}_B$

local mass flow — mass average velocity of individual molecules — $\underline{v} = \omega_A \underline{v}_A + \omega_B \underline{v}_B$

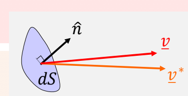
$\rho\, d\dot{V} = \rho(\,\hat{n}\cdot\underline{v})\, dS$

If, however, the molar average velocity $\underline{v}^*$ of the molecules in a mixture is calculated, a local molar flow is readily obtained:

local molar flow

$c\, d\dot{V} = c(\,\hat{n}\cdot\underline{v}^*)\, dS$

molar average velocity of individual molecules — $\underline{v}^* = x_A \underline{v}_A + x_B \underline{v}_B$



We are concerning ourselves with **sub-characteristics** of the continuum.

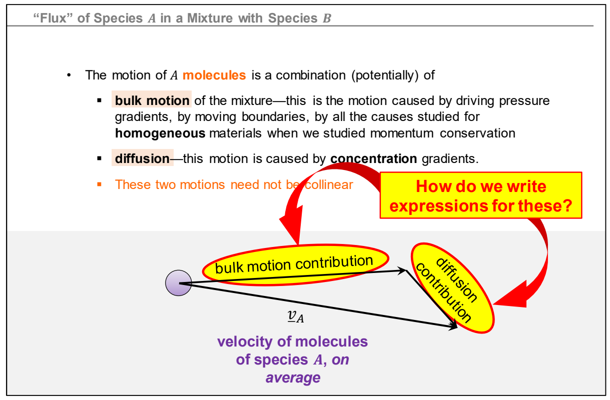
 36

So, what's the answer?

How do we write expressions for the two contributions to the average motion of molecules when diffusion is present?

Two contributions:

- ***Bulk motion***
- ***Diffusion***


"Flux" of Species A in a Mixture with Species B

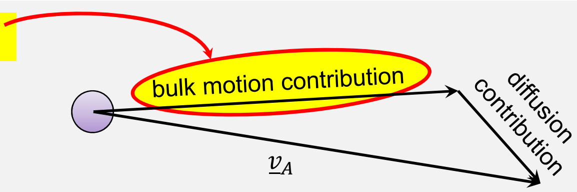
- The motion of A molecules is a combination (potentially) of
  - **bulk motion** of the mixture—this is the motion caused by driving pressure gradients, by moving boundaries, by all the causes studied for **homogeneous** materials when we studied momentum conservation
  - **diffusion**—this motion is caused by **concentration** gradients.
  - These two motions need not be collinear

 37

"Flux" of Species A in a Mixture with Species B **First Approach**

How do we write expressions for the two contributions to the average motion of molecules when diffusion is present?

Is this $\underline{v}$?



$\underline{v} = \omega_A \underline{v}_A + \omega_B \underline{v}_B$

Answer:

It can be. We have a choice as to how to write the bulk motion contribution.

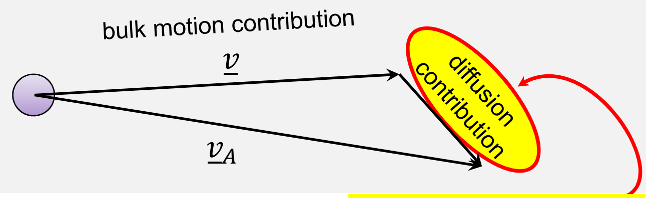
If the diffusion contribution is calculated **as the mass flux relative to $(\underline{v}_A - \underline{v})$, then the model works.**

 38

“Flux” of Species A in a Mixture with Species B

First Approach

Choose: Bulk contribution expressed as $\underline{v}$



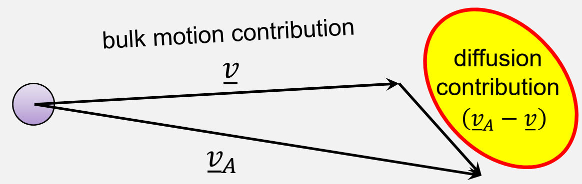
Now, what is this?

 39

“Flux” of Species A in a Mixture with Species B

First Approach

Choose: Bulk contribution expressed as $\underline{v}$



Start with mass flux:

Mass flux of $A \equiv \frac{mass\ A\ diffusing}{area \cdot time}$

$= (\underline{v}_A - \underline{v})\ \rho\ \omega_A$

volumetric flow rate per area in the direction of diffusion

$= \left(\frac{volume}{area \cdot time}\right)\left(\frac{mass\ A}{volume}\right)$

$\equiv \underline{j}_A = -\rho D_{AB} \nabla \omega_A$

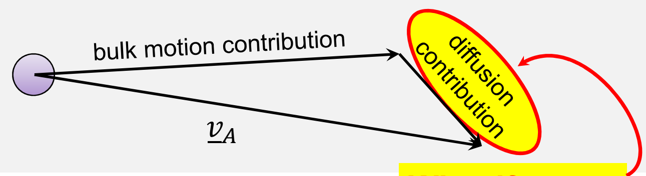
Fick’s law in mass terms

Recall in a pipe: $\frac{\dot{V}}{area} = \langle v \rangle$

 40

“Flux” of Species A in a Mixture with Species B

How do we write expressions for the two contributions to the average motion of molecules when diffusion is present?



What if I want to use a molar flux?

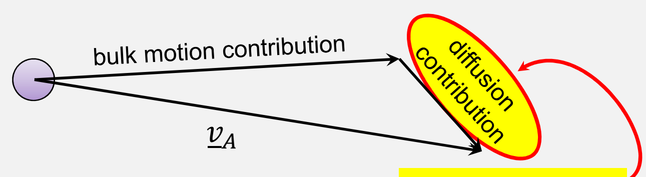
Second Approach

 41

“Flux” of Species A in a Mixture with Species B

Second Approach

How do we write expressions for the two contributions to the average motion of molecules when diffusion is present?



What if I want to use a molar flux?

Answer:

This is possible too.

To express diffusion in moles, the bulk motion contribution, however, cannot be given by the mass average velocity; instead we must use the **molar average velocity** $\underline{v}^*$.

$$\underline{v}^* = x_A \underline{v}_A + x_B \underline{v}_B$$

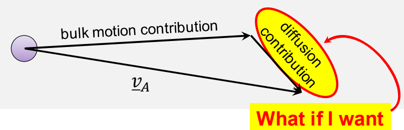
bulk molar contribution $\neq \underline{v}$

 42

"Flux" of Species A in a Mixture with Species B

Second Approach

How do we write expressions for the two contributions to the average motion of molecules when diffusion is present?



What if I want to use a molar flux?

Answer:

This is possible too.

To express diffusion in moles, the bulk motion contribution, however, cannot be given by the mass average velocity; instead we must use the **molar average velocity** $\underline{v}^*$.

bulk molar contribution $\neq \underline{v}$

To be continued

43