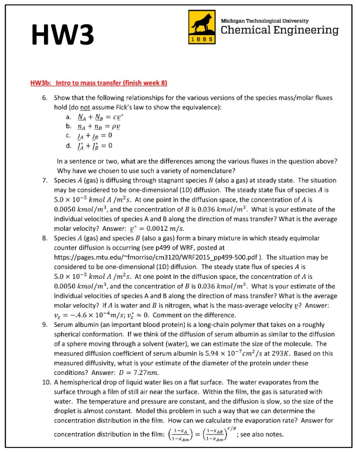
It's week 8. Next week is ***Break.***
Exam 3: Tuesday March 17
Utkarsh will be doing a ***HW/Exam prep 3/15,*** the Sunday before classes start back up.

Homework 3B:
Finish Week 8



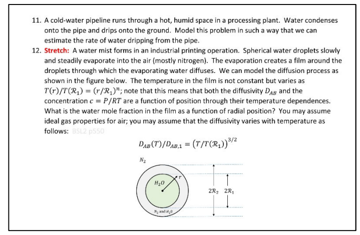
HW3

Michigan Technological University
Chemical Engineering

HW3b: Intro to mass transfer (finish week 8)

6. Show that the following relationships for the various versions of the species mass/molar fluxes hold (do not assume Fick's law to show the equivalence):
   a. $\underline{N}_A + \underline{N}_B = c\underline{v}^*$
   b. $\underline{n}_A + \underline{n}_B = \rho\underline{v}$
   c. $\underline{j}_A + \underline{j}_B = 0$
   d. $\underline{J}_A^* + \underline{J}_B^* = 0$

   In a sentence or two, what are the differences among the various fluxes in the question above? Why have we chosen to use such a variety of nomenclature?
7. Species A (gas) is diffusing through stagnant species B (also a gas) at steady state. The situation may be considered to be one-dimensional (1D) diffusion. The steady state flux of species A is $5.0 \times 10^{-5}\ kmol\ A\ /m^2s$. At one point in the diffusion space, the concentration of A is $0.0050\ kmol/m^3$, and the concentration of B is $0.036\ kmol/m^3$. What is your estimate of the individual velocities of species A and B along the direction of mass transfer? What is the average molar velocity? Answer: $\underline{v}^* = 0.0012\ m/s$.
8. Species A (gas) and species B (also a gas) form a binary mixture in which steady equimolar counter diffusion is occurring (see p499 of WRF, posted at https://pages.mtu.edu/~fmorriso/cm3120/WRF2015_pp499-500.pdf). The situation may be considered to be one-dimensional (1D) diffusion. The steady state flux of species A is $5.0 \times 10^{-5}\ kmol\ A\ /m^2s$. At one point in the diffusion space, the concentration of A is $0.0050\ kmol/m^3$, and the concentration of B is $0.036\ kmol/m^3$. What is your estimate of the individual velocities of species A and B along the direction of mass transfer? What is the average molar velocity? If A is water and B is nitrogen, what is the mass-average velocity $\underline{v}$? Answer: $v_z = -.4.6 \times 10^{-4} m/s$; $v_z^* \approx 0$. Comment on the difference.
9. Serum albumin (an important blood protein) is a long-chain polymer that takes on a roughly spherical conformation. If we think of the diffusion of serum albumin as similar to the diffusion of a sphere moving through a solvent (water), we can estimate the size of the molecule. The measured diffusion coefficient of serum albumin is $5.94 \times 10^{-7} cm^2/s$ at $293K$. Based on this measured diffusivity, what is your estimate of the diameter of the protein under these conditions? Answer: $D = 7.27nm$.
10. A hemispherical drop of liquid water lies on a flat surface. The water evaporates from the surface through a film of still air near the surface. Within the film, the gas is saturated with water. The temperature and pressure are constant, and the diffusion is slow, so the size of the droplet is almost constant. Model this problem in such a way that we can determine the concentration distribution in the film. How can we calculate the evaporation rate? Answer for concentration distribution in the film: $\left(\frac{1-x_A}{1-x_{A\infty}}\right) = \left(\frac{1-x_{AR}}{1-x_{A\infty}}\right)^{r/R}$; see also notes.



11. A cold-water pipeline runs through a hot, humid space in a processing plant. Water condenses onto the pipe and drips onto the ground. Model this problem in such a way that we can estimate the rate of water dripping from the pipe.
12. **Stretch:** 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 below. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$; note that this means that both the diffusivity D_{AB} and the concentration $c = P/RT$ are a function of position through their temperature dependences. 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: BSL2 p550

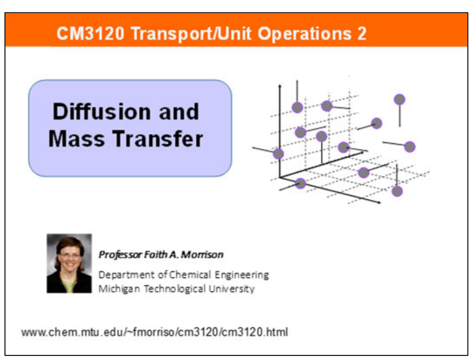
$$D_{AB}(T)/D_{AB,1} = \left(T/T(\mathcal{R}_1)\right)^{3/2}$$

Exam 3 topics:
- ***Lectures 9-12 and 1-11 and all prereqs***
- ***HW3a 3b, also HW1, HW2 and prereqs***

1

Now, Cycling Back:

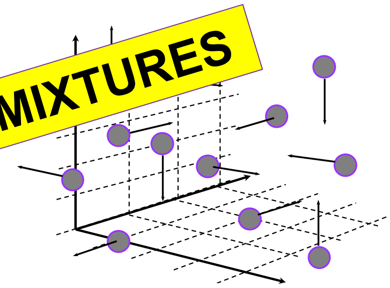
Diffusion and Mass Transfer



2

CM3120 Transport/Unit Operations 2

Diffusion and Mass Transfer in MIXTURES



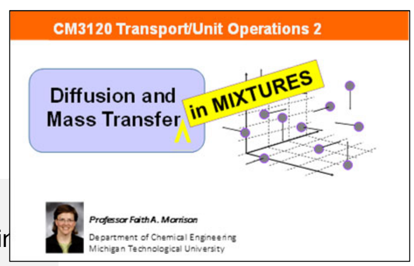
Professor Faith A. Morrison
Department of Chemical Engineering
Michigan Technological University

We began a few weeks ago…

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

 3

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



Summary:

- Occurs in mixtures; this complicates thin
- 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

 4

QUICK START

Recap:

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 →

5

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	$c\left(\frac{\partial x_A}{\partial t} + \underline{v}^*\cdot\nabla x_A\right) = -\nabla\cdot\underline{J}_A^* + (x_B R_A - x_A R_B)$ $= cD_{AB}\nabla^2 x_A + (x_B R_A - x_A R_B)$
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 →

6

QUICK START

Recap:

Various quantities in diffusion and mass transfer

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

$\underline{j}_A \equiv$ **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

7

QUICK START

Recap:

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

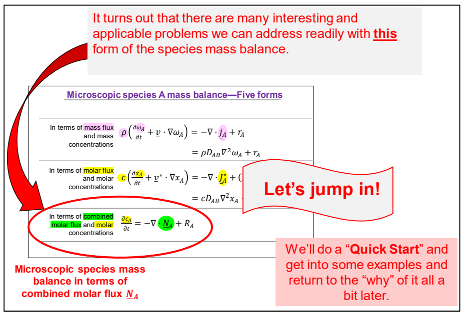
8

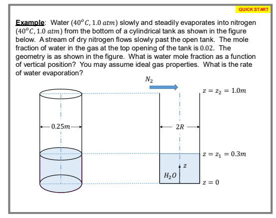
QUICK START

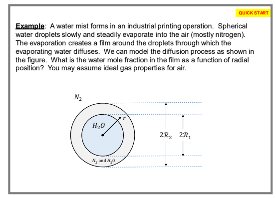
We skipped to one version of the *Species A mass balance* (and Fick's law) and got some practice.

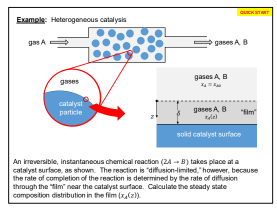
$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

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









9

QUICK START

Recap: Introduction to Diffusion and Mass Transfer in Mixtures

Recurring Modeling Assumptions in Diffusion

- Near a liquid-gas interface, the region in the gas near the liquid is a film where 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, $\underline{N}_A = 0$.
- If A diffuses through stagnant B, $\underline{N}_B = 0$.
- If, for example, two moles of A diffuse to a surface at which a rapid, irreversible reaction coverts it to one mole of B, then at steady state $-0.5\underline{N}_A = \underline{N}_B$.
- Because diffusion is slow, we can make a quasi-steady-state assumption
- Homogeneous reactions appear in the mass balance; heterogeneous reactions appear in the boundary conditions
- If a binary mixture of A and B are undergoing steady equimolar counter diffusion, $\underline{N}_A = -\underline{N}_B$. (coming)
-
-

10

QUICK START

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

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

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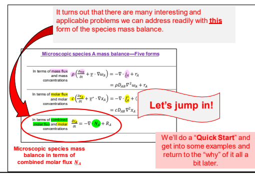

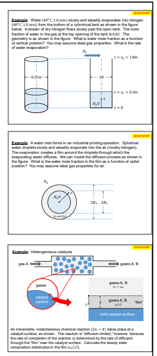

The **QUICK START** has perhaps led to the impression that the ***combined molar flux*** version is all we need to address problems in mass transfer…

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.

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?

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

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

Introduction to Diffusion and Mass Transfer in Mixtures

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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

13

Transport Laws, up to now:

Part I: Momentum Transfer

Momentum transfer:

$$\underbrace{\tau_{21} = (-\tilde{\tau}_{21})}_{\text{momentum flux}} = -\mu\underbrace{\left(\frac{dv_1}{dx_2}\right)}_{\text{velocity gradient}}$$

μ – viscosity

Newton's law of viscosity

Part II: Heat Transfer

Heat transfer:

$$\underbrace{\frac{q_x}{A}}_{\text{heat flux}} = -k\underbrace{\frac{dT}{dx}}_{\text{temperature gradient}}$$

k – thermal conductivity

Fourier's law of conduction

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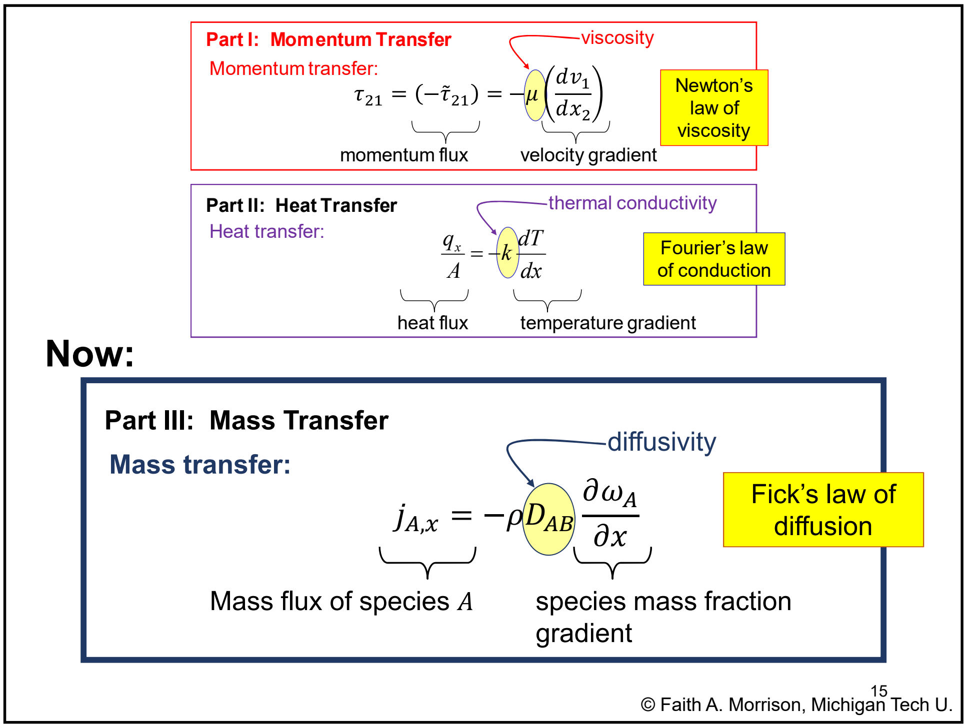
Part I: Momentum Transfer
Momentum transfer:
viscosity
$\tau_{21} = (-\tilde{\tau}_{21}) = -\mu\left(\frac{dv_1}{dx_2}\right)$
momentum flux
velocity gradient
Newton's law of viscosity
Part II: Heat Transfer
Heat transfer:
thermal conductivity
$\frac{q_x}{A} = -k\frac{dT}{dx}$
heat flux
temperature gradient
Fourier's law of conduction
Now:
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
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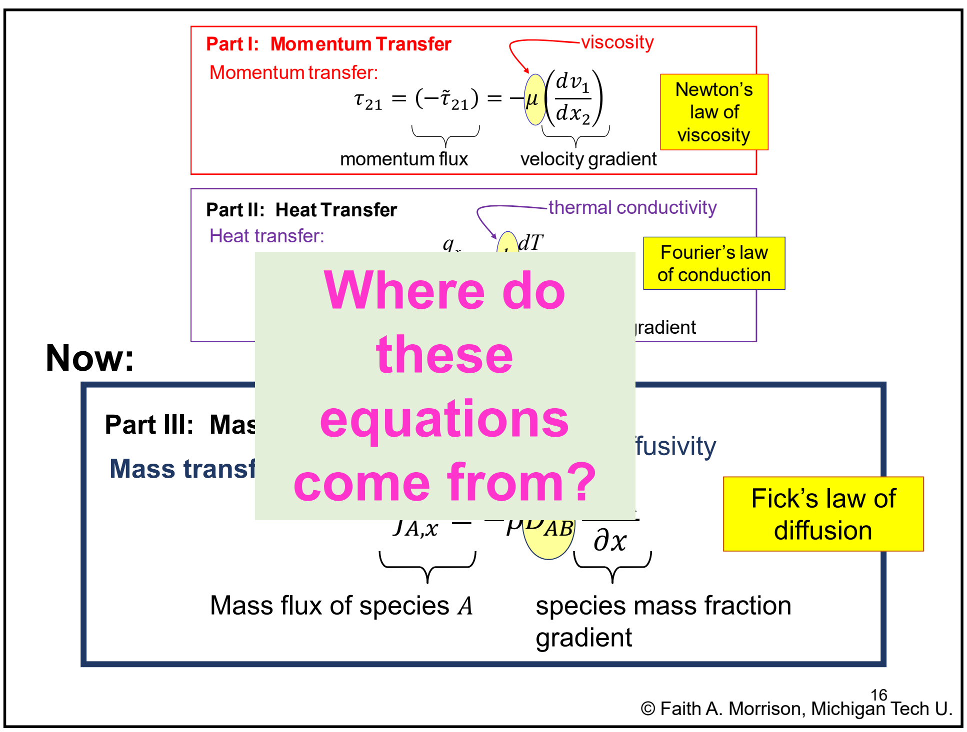
Part I: Momentum Transfer
Momentum transfer:
viscosity
$\tau_{21} = (-\tilde{\tau}_{21}) = -\mu\left(\frac{dv_1}{dx_2}\right)$
momentum flux
velocity gradient
Newton's law of viscosity
Part II: Heat Transfer
Heat transfer:
thermal conductivity
Fourier's law of conduction
Where do these equations come from?
Now:
Part III: Mas
Mass transf
Mass flux of species A
species mass fraction gradient
Fick's law of diffusion
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The Physics of the Transport Laws

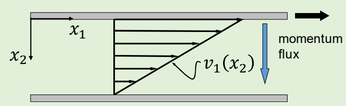
Part I: Momentum Transfer

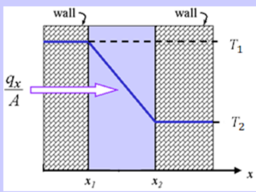
Momentum transfer:

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

momentum flux; viscosity (μ); 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 (k); temperature gradient

Fourier's law of conduction

Part III: Mass Transfer

Mass transfer:

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

Mass flux of species A; diffusivity (D_{AB}); species mass fraction gradient

Fick's law of diffusion

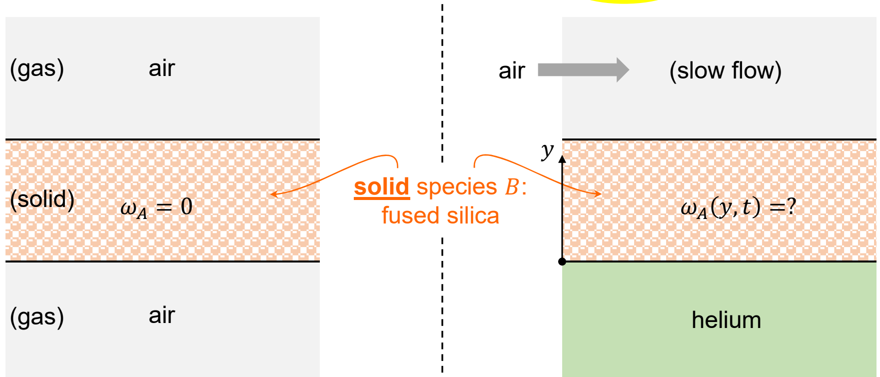
Where does *this* equation come from?

 17

Simple One-dimensional Species Mass Diffusion

What is the physics behind the mass diffusion transport law?

Initially: | ***Suddenly*** $(t = 0)$:



solid species B: fused silica

gas species A: helium

Assumptions:

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

BSL2, p514

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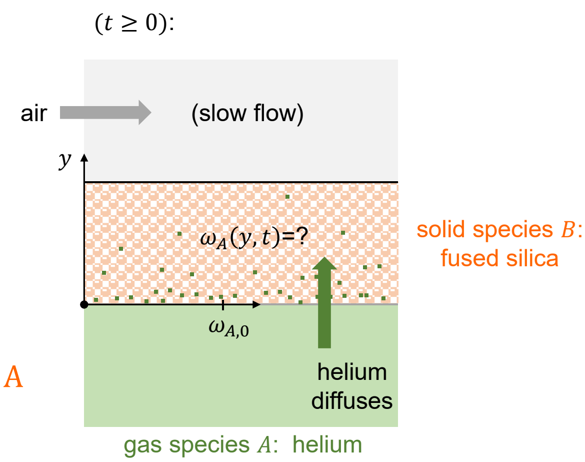
Simple One-dimensional Species Mass Diffusion

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



ω_A = mass fraction of A

BSL2, p514

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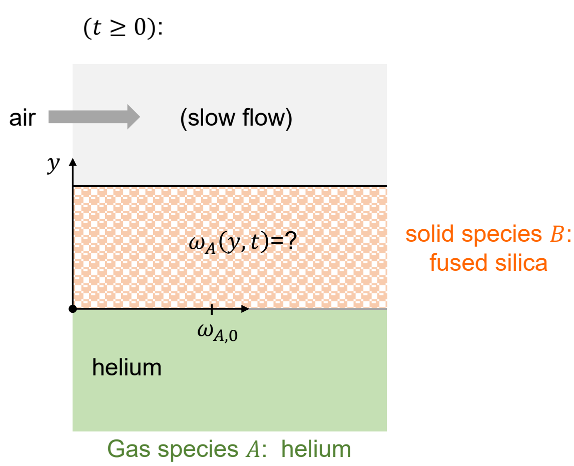
Simple One-dimensional Species Mass Diffusion

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



You try.

BSL2, p514

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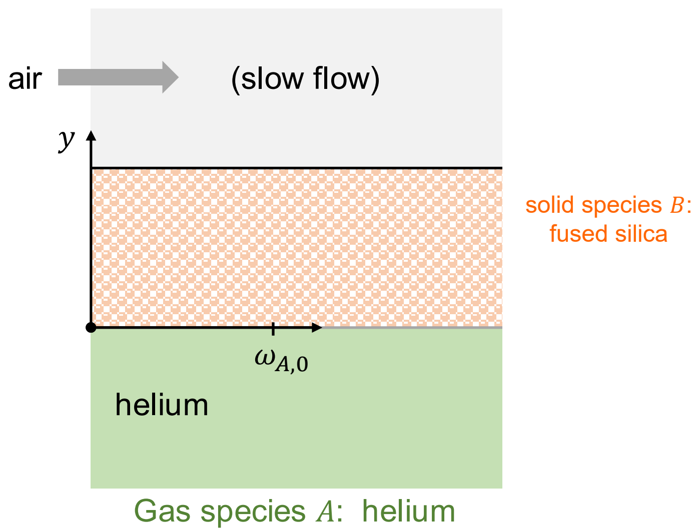
Simple One-dimensional Species Mass Diffusion

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

$(t \geq 0)$:



BSL2, p514

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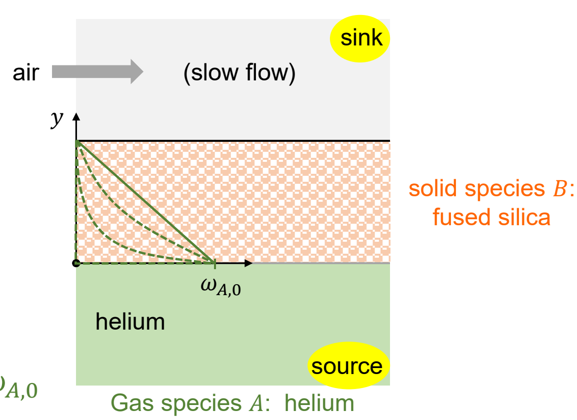
Simple One-dimensional Species Mass Diffusion

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

Suddenly $(t = 0)$:



At steady state,

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

BSL2, p514

22

Simple One-dimensional Species Mass Diffusion

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

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

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

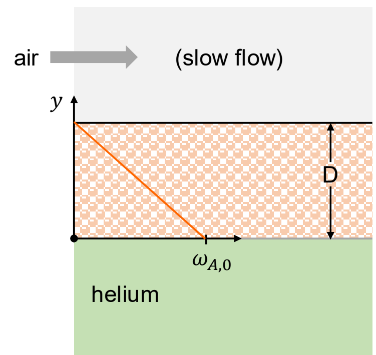
Fick's law of diffusion

(in terms of mass flux)

D_{AB} = Diffusion coefficient of A through B

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

Suddenly $(t = 0)$:



Gas species A: helium

BSL2, p514

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Simple One-dimensional Species Mass Diffusion

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

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

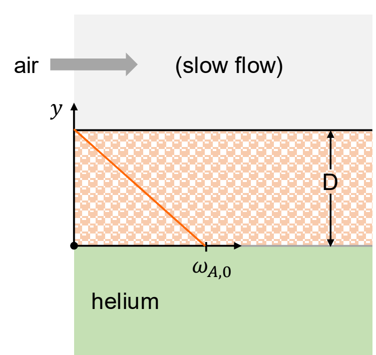
Fick's law of diffusion

(in terms of mass flux)

D_{AB} = Diffusion coefficient of A through B

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

Suddenly $(t = 0)$:



Gas species A: helium

BSL2, p514

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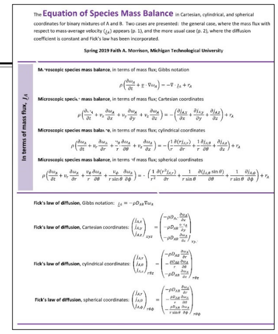
Law of Species Diffusion



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

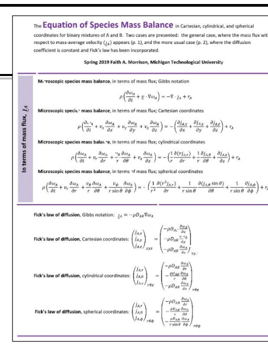
Gibbs notation: $\underline{j}_A = -\rho \mathrm{D}_{\mathrm{AB}} \nabla \omega_A$

Fick's law

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

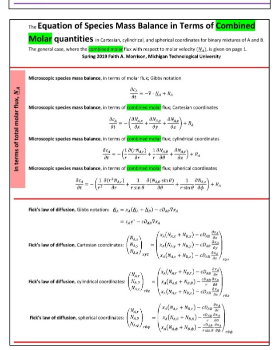
- Mass diffuses flows **down** a concentration gradient
- Flux is proportional to magnitude of concentration gradient

Law of Species Diffusion



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

But *not* the one we have been using!



Law of Species Diffusion

***QUESTION*:**

Why so many versions of species A flux?

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**.

***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.

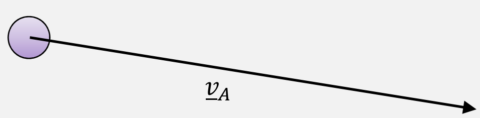
"Flux" of Species A in a Mixture with Species B

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:

$$\underline{v}_A = \frac{1}{n_T}\sum_{i=1}^{n_T} \underline{v}_{A,i} \qquad \textit{(a regular average)}$$



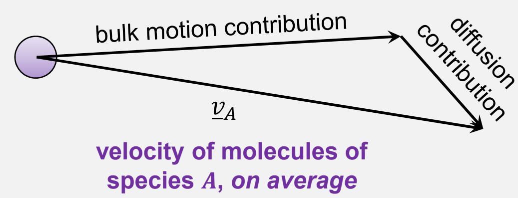
velocity of molecules of species A, *on average*

(in a region of space)

- 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 primarily 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**



(in a region of space)

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

- The motion of A **molecules** is a combination (potentially) of
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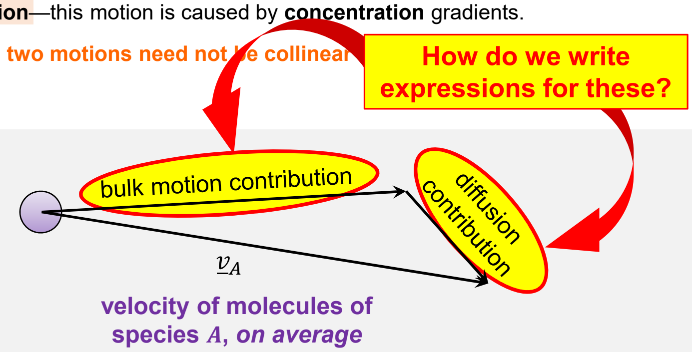
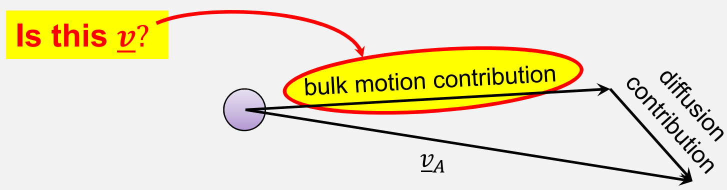


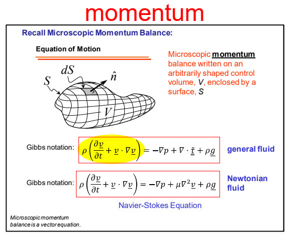
(in a region of space)

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



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

momentum


Recall Microscopic Momentum Balance:

Equation of Motion

Microscopic **momentum** balance written on an arbitrarily shaped control volume, V, enclosed by a surface, S

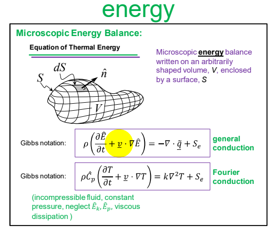
Gibbs notation: $\rho\left(\frac{\partial \underline{v}}{\partial t} + \underline{v}\cdot\nabla\underline{v}\right) = -\nabla p + \nabla\cdot\underline{\underline{\tilde{\tau}}} + \rho\underline{g}$ general fluid

Gibbs notation: $\rho\left(\frac{\partial \underline{v}}{\partial t} + \underline{v}\cdot\nabla\underline{v}\right) = -\nabla p + \mu\nabla^2\underline{v} + \rho\underline{g}$ Newtonian fluid

Navier-Stokes Equation

Microscopic momentum balance is a vector equation.

energy


Microscopic Energy Balance:

Equation of Thermal Energy

Microscopic **energy** balance written on an arbitrarily shaped volume, V, enclosed by a surface, S

Gibbs notation: $\rho\left(\frac{\partial \hat{E}}{\partial t} + \underline{v}\cdot\nabla\hat{E}\right) = -\nabla\cdot\underline{\tilde{q}} + S_e$ general conduction

Gibbs notation: $\rho\hat{C}_p\left(\frac{\partial T}{\partial t} + \underline{v}\cdot\nabla T\right) = k\nabla^2 T + S_e$ Fourier conduction

(incompressible fluid, constant pressure, neglect $\hat{E}_k, \hat{E}_p$, viscous dissipation)

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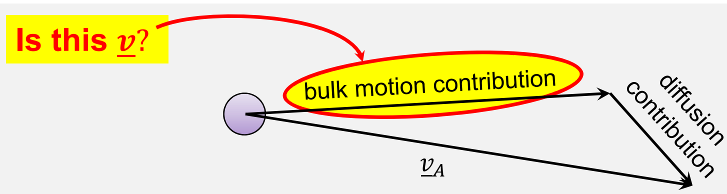
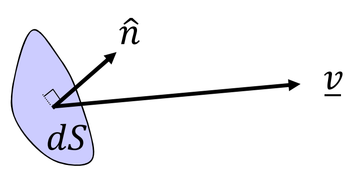
"Flux" of Species A in a Mixture with Species B



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?

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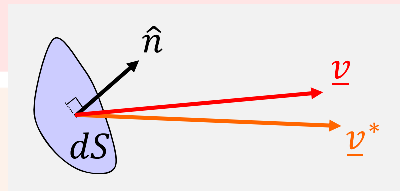
"Flux" of Species A in a Mixture with Species B

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

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

(continuum is divided into mass "particles")



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

local molar flow

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

molar average velocity of individual molecules

(continuum is divided into molar "particles")

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

 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

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

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

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 ***is not the same:***

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: $\underline{v}^*$ = the molar average velocity

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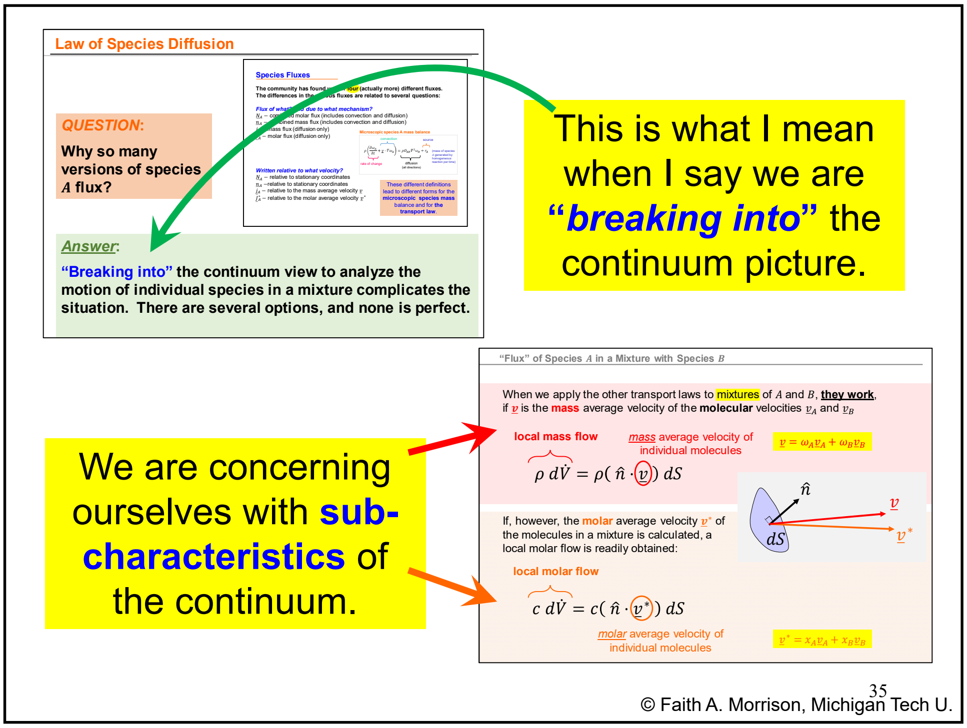
Law of Species Diffusion
QUESTION:
Why so many versions of species A flux?
Species Fluxes
Answer:
"Breaking into" the continuum view to analyze the motion of individual species in a mixture complicates the situation. There are several options, and none is perfect.
This is what I mean when I say we are "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 v is the mass average velocity of the molecular velocities v_A and v_B
local mass flow
mass average velocity of individual molecules
$v = \omega_A v_A + \omega_B v_B$
$\rho \, d\dot{V} = \rho(\hat{n} \cdot v)\, dS$
$\hat{n}$
dS
If, however, the molar average velocity v^* of the molecules in a mixture is calculated, a local molar flow is readily obtained:
local molar flow
$c \, d\dot{V} = c(\hat{n} \cdot v^*)\, dS$
molar average velocity of individual molecules
$v^* = x_A v_A + x_B v_B$
We are concerning ourselves with sub-characteristics of the continuum.
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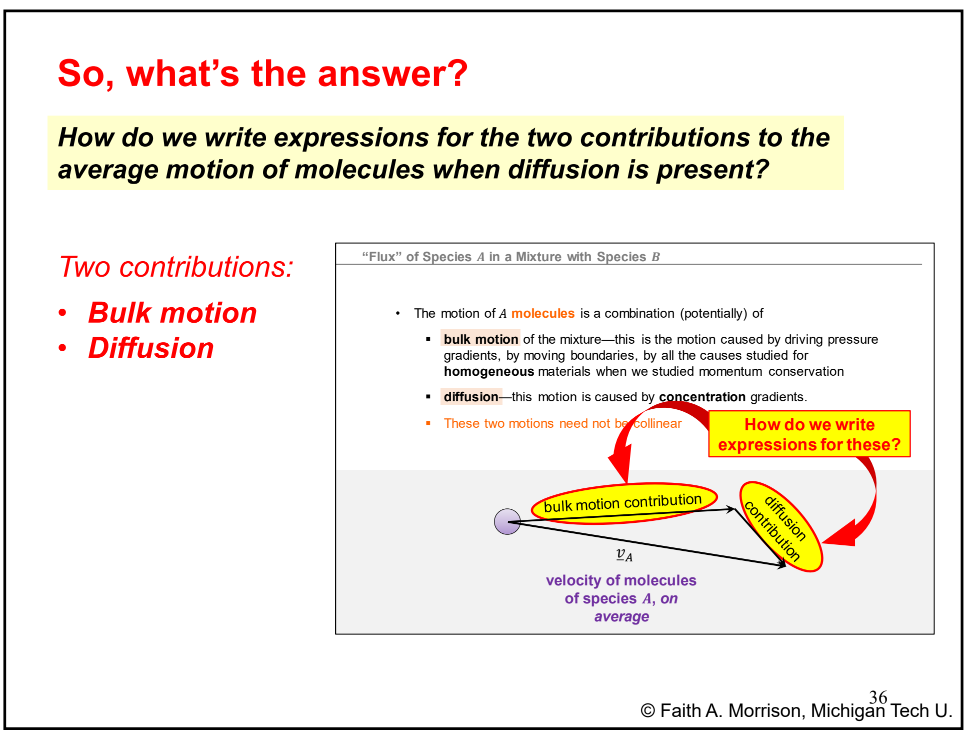
So, what's the answer?
How do we write expressions for the two contributions to the average motion of molecules when diffusion is present?
Two contributions:
• Bulk motion
• Diffusion
"Flux" of Species A in a Mixture with Species B
• The motion of A molecules is a combination (potentially) of
▪ bulk 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
How do we write expressions for these?
bulk motion contribution
diffusion contribution
v_A
velocity of molecules of species A, on average
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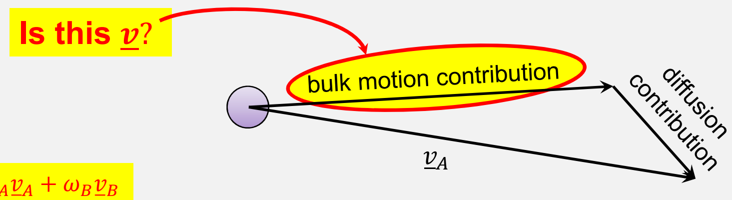
"Flux" of Species A in a Mixture with Species B

First Approach

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



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

Answer:

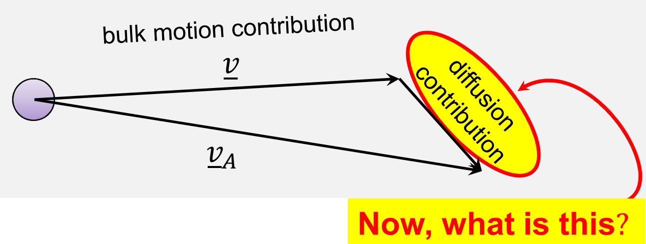
It can be. We have a choice as to how to write the bulk motion contribution.

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

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

First Approach

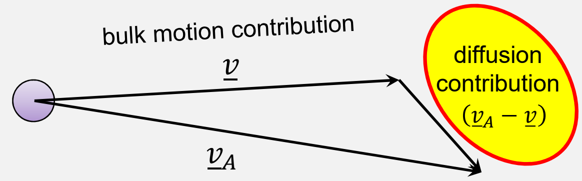
Choose: Bulk contribution expressed as $\underline{v}$



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

First Approach

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



Start with mass flux:

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

$$= (\underline{v}_A - \underline{v})\,\rho\,\omega_A \equiv \underline{j}_A = -\rho D_{AB} \nabla \omega_A$$

Fick's law in mass terms

volumetric flow rate per area in the direction of diffusion

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

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

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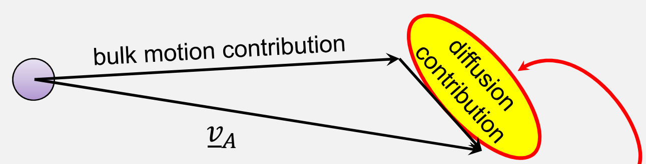
“Flux” of Species A in a Mixture with Species B

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

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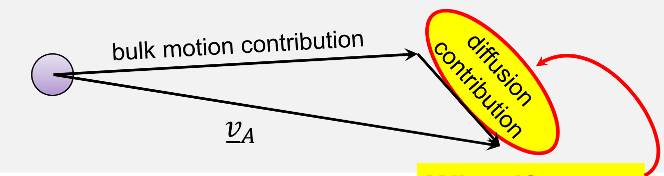
"Flux" of Species A in a Mixture with Species B

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 <u>moles</u>, 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 $\neq \underline{v}$

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"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?
bulk motion contribution
diffusion contribution
$\underline{v}_A$
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

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