

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**



**HW3a: Intro to mass transfer (finish week 8)**

- Show that the following relationships for the various versions of the species/molar fluxes hold (do not assume Fick's law to show the equivalence):
  - $D_{12} = D_{21} = D^*$
  - $D_{12} + D_{21} = D^*$
  - $J_1 + J_2 = 0$
  - $\bar{J}_1 + \bar{J}_2 = 0$
- 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?
- 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  $5.0 \times 10^{-7}$  kmol A / m<sup>2</sup> s. At one point in the diffusion space, the concentration of A is 0.0050 kmol/m<sup>3</sup> and the concentration of B is 0.036 kmol/m<sup>3</sup>. 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:  $v = 0.0012$  m/s.
- Species A (gas) and species B (also a gas) form a binary mixture in which steady equimolar counter diffusion is occurring (see p499 of WRR, posted at [https://pages.mtu.edu/~fmorriso/cm3120/WRR2013\\_pp499-500.pdf](https://pages.mtu.edu/~fmorriso/cm3120/WRR2013_pp499-500.pdf)). The situation may be considered to be one-dimensional (1D) diffusion. The steady state flux of species A is  $5.0 \times 10^{-7}$  kmol A / m<sup>2</sup> s. At one point in the diffusion space, the concentration of A is 0.0050 kmol/m<sup>3</sup> and the concentration of B is 0.036 kmol/m<sup>3</sup>. 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? Answer:  $v_A = -4.6 \times 10^{-7}$  m/s;  $v_B = 0$ . Comment on the difference.
- Seven 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  $5.8 \times 10^{-10}$  m<sup>2</sup>/s at 29°C. Based on this measured diffusivity, what is your estimate of the diameter of the protein under these conditions? Answer:  $D = 7.27$  nm.
- 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:  $\frac{r^2 - R^2}{R^2} = \frac{C - C_s}{C_\infty - C_s}$ ; see also notes.

- 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.
- 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  $T(r)/T(R_s) = (r/R_s)^2$ ; note that this means that both the diffusivity  $D_{12}$  and the concentration  $c = P/RT$  are a function of position through their temperature dependence. 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:  $D_{12}(T)/D_{12}(T_s) = (T/T_s)^{1.75}$

**Exam 3 topics:**

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

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# Now, Cycling Back:

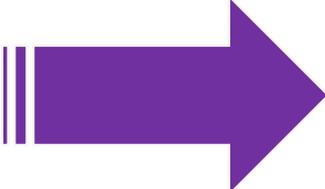
## Diffusion and Mass Transfer

**CM3120 Transport/Unit Operations 2**

**Diffusion and Mass Transfer**

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

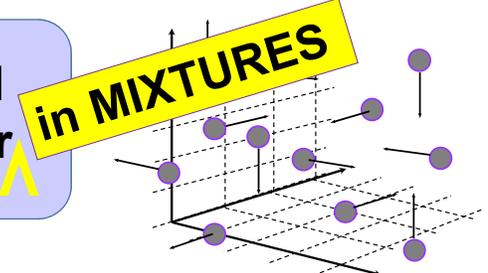
[www.chem.mtu.edu/~fmorriso/cm3120/cm3120.html](http://www.chem.mtu.edu/~fmorriso/cm3120/cm3120.html)



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**CM3120 Transport/Unit Operations 2**

## Diffusion and Mass Transfer





**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](http://www.chem.mtu.edu/~fmorriso/cm3120/cm3120.html)

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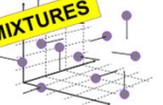
**We first introduced the topic of diffusion and mass transfer a few weeks ago...**

**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...

CM3120 Transport/Unit Operations 2

### Diffusion and Mass Transfer





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

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*

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**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?**

$\bar{N}_A$  – combined molar flux (includes both convection and diffusion)  
 $\bar{m}_A$  – combined mass flux (includes both convection and diffusion)  
 $\bar{j}_A$  – mass flux (diffusion only)  
 $\bar{J}_A$  – molar flux (diffusion only)

**Microscopic species A mass balance**

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

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

**Written relative to what velocity?**

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

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

**QUICK START**

These different fluxes are a significant complication.

➔

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

➔

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**Recap:**

**Microscopic species A mass balance—Five forms**

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

**QUICK START**

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

➔

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**Recap:**

**Various quantities in diffusion and mass transfer**

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

$j_A \equiv$  **mass flux** of species  $A$  relative to a mixture's **mass average velocity**,  $v$   
 $= \rho_A(v_A - v)$   
 $j_A + j_B = 0$ , i.e. these fluxes are measured relative to the mixture's center of mass

$n_A \equiv \rho_A v_A = j_A + \rho_A v =$  **combined mass flux** relative to **stationary coordinates**  
 $n_A + n_B = \rho v$

$J_A \equiv$  **molar flux** relative to a mixture's **molar average velocity**,  $v^*$   
 $= c_A(v_A - v^*)$   
 $J_A + J_B = 0$

$N_A \equiv c_A v_A = J_A + c_A v^* =$  **combined molar flux** relative to **stationary coordinates**  
 $N_A + N_B = c v^*$

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

**QUICK START**

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

➔

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**Recap:**

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

Mass flux

 $j_A = -\rho D_{AB} \nabla \omega_A$

Molar flux

 $J_A = -c D_{AB} \nabla x_A$

Combined molar flux

 $N_A = x_A(N_A + N_B) - c D_{AB} \nabla x_A$

FRONT  
[pages.mtu.edu/~fmorriso/cm3120/Homeworks\\_Reading.s.html](http://pages.mtu.edu/~fmorriso/cm3120/Homeworks_Reading.s.html)

**QUICK START**

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

➔

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**QUICK START**

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

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

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

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:  $\rho \left( \frac{d\omega_A}{dt} + \mathbf{y} \cdot \nabla \omega_A \right) = -\nabla \cdot \underline{j}_A + r_A$   
 $= \rho D_{AB} \nabla^2 \omega_A + r_A$

In terms of molar flux and molar concentrations:  $c \left( \frac{dx_A}{dt} + \mathbf{y} \cdot \nabla x_A \right) = -\nabla \cdot \underline{J}_A + R_A$   
 $= cD_{AB} \nabla^2 x_A + R_A$

In terms of **molar flux and molar concentrations**:  $\underline{J}_A = -\nabla x_A + \mathbf{y} x_A$

In terms of **combined molar flux and molar concentrations**:  $\underline{N}_A = -\nabla x_A + \mathbf{y} x_A + R_A$

**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.

**Example:** Water (at 20°C, 1.0 atm) slowly and steadily evaporates into nitrogen (N<sub>2</sub>, 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?

**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.

**Example:** Heterogeneous catalysis

An irreversible, instantaneous chemical reaction (2A → B) takes place at a catalyst surface, as shown. The reaction is "diffusion-limited," however, because the rate of completion of the reaction is determined by the rate of diffusion through the "film" near the catalyst surface. Calculate the steady state composition distribution in the film (p, x, A).

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**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 converts 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)
- 
- 

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**QUICK START**

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

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

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

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!**

We'll do a "Quick Start" and get into some exercises and return to the "why" of it all a centered later this fall.

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.

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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)
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- $\underline{J}_A$  – mass flux (diffusion only)
- $\underline{j}_A$  – molar flux (diffusion only)

**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.

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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?

We cycle back now to return to this discussion

**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?**

- $N_A$  – combined molar flux (includes convection and diffusion)
- $n_A$  – combined mass flux (includes convection and diffusion)
- $J_A$  – mass flux (diffusion only)
- $\tilde{J}_A$  – molar flux (diffusion only)

**Written relative to what velocity?**

- $N_A$  – relative to stationary coordinates
- $n_A$  – relative to stationary coordinates
- $J_A$  – relative to the mass average velocity  $\bar{v}$
- $\tilde{J}_A$  – relative to the molar average velocity  $\bar{v}'$

**Microscopic species A mass balance**

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

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

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



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Transport Laws, up to now:

**Part I: Momentum Transfer**

Momentum transfer:

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

momentum flux      velocity gradient      viscosity

Newton's law of viscosity

**Part II: Heat Transfer**

Heat transfer:

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

heat flux      temperature gradient      thermal conductivity

Fourier's law of conduction

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**Part I: Momentum Transfer**

Momentum transfer:

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

Newton's law of viscosity

**Part II: Heat Transfer**

Heat transfer:

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

Fourier's law of conduction

**Now:**

**Part III: Mass Transfer**

Mass transfer:

$$j_{A,x} = -\underbrace{\rho}_{\text{diffusivity}} \underbrace{D_{AB}}_{\text{diffusivity}} \underbrace{\frac{\partial \omega_A}{\partial x}}_{\text{species mass fraction gradient}}$$

Fick's law of diffusion

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**Part I: Momentum Transfer**

Momentum transfer:

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

Newton's law of viscosity

**Part II: Heat Transfer**

Heat transfer:

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

Fourier's law of conduction

**Now:**

**Part III: Mass Transfer**

Mass transfer:

$$j_{A,x} = -\underbrace{\rho}_{\text{diffusivity}} \underbrace{D_{AB}}_{\text{diffusivity}} \underbrace{\frac{\partial \omega_A}{\partial x}}_{\text{species mass fraction gradient}}$$

Fick's law of diffusion

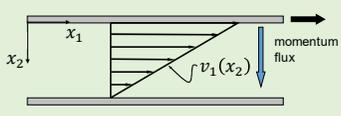
Where do these equations come from?

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### The Physics of the Transport Laws

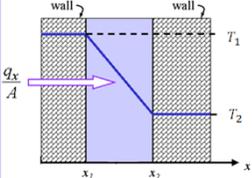
**Part I: Momentum Transfer**  
 Momentum transfer:  

$$\tau_{21} = (-\tilde{\tau}_{21}) = -\mu \left( \frac{dv_1}{dx_2} \right)$$
 momentum flux      velocity gradient      viscosity      **Newton's law of viscosity**



**Part II: Heat Transfer**  
 Heat transfer:  

$$\frac{q_x}{A} = -k \frac{dT}{dx}$$
 heat flux      temperature gradient      thermal conductivity      **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      species mass fraction gradient      diffusivity      **Fick's law of diffusion**

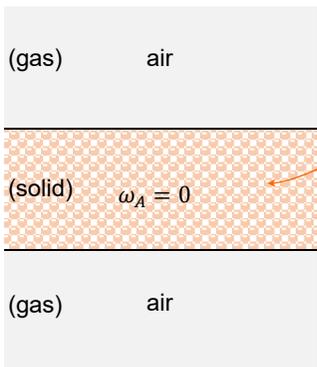
← Where does this equation come from?

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### Simple One-dimensional Species Mass Diffusion

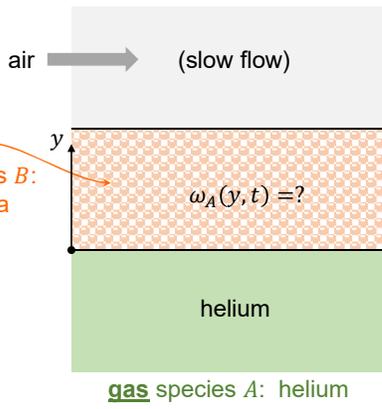
What is the physics behind the mass diffusion transport law?

Initially:



$\omega_A = 0$

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



$\omega_A(y, t) = ?$

gas species A: helium

solid species B: fused silica

Assumptions:

- wide, deep  $\Rightarrow$  1D diffusion
- no reaction
- species B not moving

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Simple One-dimensional Species Mass Diffusion

( $t \geq 0$ ):

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

$\omega_A =$  mass fraction of A

The diagram shows a vertical cross-section of a diffusion system. At the top, a grey region represents air with a horizontal arrow pointing right labeled '(slow flow)'. Below this is a red checkered region representing a solid species B, fused silica. A vertical y-axis is shown on the left, with the origin at the interface between the solid and gas layers. The mass fraction in the solid is labeled  $\omega_A(y, t) = ?$ . Below the solid is a green region representing gas species A, helium. A horizontal arrow at the interface points right, labeled  $\omega_{A,0}$ . A vertical arrow points up from the gas into the solid, labeled 'helium diffuses'. The text 'gas species A: helium' is at the bottom of the green region.

air (slow flow)

$y$

$\omega_A(y, t) = ?$

solid species B: fused silica

$\omega_{A,0}$

helium diffuses

gas species A: helium

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Simple One-dimensional Species Mass Diffusion

( $t \geq 0$ ):

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

**You try.**

The diagram is identical to the one above, showing a vertical cross-section of a diffusion system. At the top, a grey region represents air with a horizontal arrow pointing right labeled '(slow flow)'. Below this is a red checkered region representing a solid species B, fused silica. A vertical y-axis is shown on the left, with the origin at the interface between the solid and gas layers. The mass fraction in the solid is labeled  $\omega_A(y, t) = ?$ . Below the solid is a green region representing gas species A, helium. A horizontal arrow at the interface points right, labeled  $\omega_{A,0}$ . The text 'helium' is written inside the green region, and 'Gas species A: helium' is at the bottom of the green region.

air (slow flow)

$y$

$\omega_A(y, t) = ?$

solid species B: fused silica

$\omega_{A,0}$

helium

Gas species A: helium

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Simple One-dimensional Species Mass Diffusion

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

( $t \geq 0$ ):

air (slow flow)

solid species B: fused silica

helium  
Gas species A: helium

$\omega_{A,0}$

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Simple One-dimensional Species Mass Diffusion

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

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

air (slow flow) sink

solid species B: fused silica

helium source  
Gas species A: helium

$\omega_{A,0}$

At steady state,  

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

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Simple One-dimensional Species Mass Diffusion

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

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

**Suddenly (t = 0):**

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

**Suddenly (t = 0):**

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### Law of Species Diffusion

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

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

Fick's law 
$$\underline{j}_A = \begin{pmatrix} -\rho D_{AB} \frac{\partial \omega_A}{\partial x} \\ -\rho D_{AB} \frac{\partial \omega_A}{\partial y} \\ -\rho D_{AB} \frac{\partial \omega_A}{\partial z} \end{pmatrix}_{xyz}$$

**The Equation of Species Mass Balance** in Cartesian, cylindrical, and spherical coordinates for steady, laminar flow. The general case, where the mass flux with respect to mass average velocity  $\underline{v}_m$  appears in (1), and the more usual case (2), where the diffusion coefficient is constant and  $\underline{v}_m$  has been incorporated.

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

$$\rho \frac{D\omega_A}{Dt} + \nabla \cdot (\rho \omega_A \underline{v}_m) - \nabla \cdot \underline{j}_A = \dot{r}_A$$

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

$$\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v}_m \cdot \nabla \omega_A + \omega_A \nabla \cdot \underline{v}_m \right) - \left( \frac{\partial}{\partial x} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial y} \right) + \frac{\partial}{\partial z} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial z} \right) \right) + \dot{r}_A$$

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

$$\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v}_m \cdot \nabla \omega_A + \omega_A \nabla \cdot \underline{v}_m \right) - \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho D_{AB} \frac{\partial \omega_A}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial z} \right) \right) + \dot{r}_A$$

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

$$\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v}_m \cdot \nabla \omega_A + \omega_A \nabla \cdot \underline{v}_m \right) - \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho D_{AB} \frac{\partial \omega_A}{\partial r} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \rho D_{AB} \frac{\partial \omega_A}{\partial \theta} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial \phi} \right) \right) + \dot{r}_A$$

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

**Fick's law of diffusion, Cartesian coordinates**  $\begin{pmatrix} j_{Ax} \\ j_{Ay} \\ j_{Az} \end{pmatrix} = -\rho D_{AB} \begin{pmatrix} \frac{\partial \omega_A}{\partial x} \\ \frac{\partial \omega_A}{\partial y} \\ \frac{\partial \omega_A}{\partial z} \end{pmatrix}$

**Fick's law of diffusion, cylindrical coordinates**  $\begin{pmatrix} j_{Ar} \\ j_{A\theta} \\ j_{Az} \end{pmatrix} = -\rho D_{AB} \begin{pmatrix} \frac{\partial \omega_A}{\partial r} \\ \frac{1}{r} \frac{\partial \omega_A}{\partial \theta} \\ \frac{\partial \omega_A}{\partial z} \end{pmatrix}$

**Fick's law of diffusion, spherical coordinates**  $\begin{pmatrix} j_{Ar} \\ j_{A\theta} \\ j_{A\phi} \end{pmatrix} = -\rho D_{AB} \begin{pmatrix} \frac{\partial \omega_A}{\partial r} \\ \frac{1}{r} \frac{\partial \omega_A}{\partial \theta} \\ \frac{1}{r \sin \theta} \frac{\partial \omega_A}{\partial \phi} \end{pmatrix}$

- 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!

**The Equation of Species Mass Balance** in Cartesian, cylindrical, and spherical coordinates for steady, laminar flow. The general case, where the mass flux with respect to mass average velocity  $\underline{v}_m$  appears in (1), and the more usual case (2), where the diffusion coefficient is constant and  $\underline{v}_m$  has been incorporated.

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

$$\rho \frac{D\omega_A}{Dt} + \nabla \cdot (\rho \omega_A \underline{v}_m) - \nabla \cdot \underline{j}_A = \dot{r}_A$$

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

$$\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v}_m \cdot \nabla \omega_A + \omega_A \nabla \cdot \underline{v}_m \right) - \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho D_{AB} \frac{\partial \omega_A}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial z} \right) \right) + \dot{r}_A$$

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

$$\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v}_m \cdot \nabla \omega_A + \omega_A \nabla \cdot \underline{v}_m \right) - \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho D_{AB} \frac{\partial \omega_A}{\partial r} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \rho D_{AB} \frac{\partial \omega_A}{\partial \theta} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial \phi} \right) \right) + \dot{r}_A$$

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**The Equation of Species Mass Balance in Terms of Molar Fluxes** in Cartesian, cylindrical, and spherical coordinates for steady, laminar flow. The general case, where the molar flux with respect to molar velocity  $\underline{v}_m$  appears in (1), is given on page 1.

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

$$\rho \frac{D\omega_A}{Dt} + \nabla \cdot (\rho \omega_A \underline{v}_m) - \nabla \cdot \underline{j}_A = \dot{r}_A$$

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

$$\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v}_m \cdot \nabla \omega_A + \omega_A \nabla \cdot \underline{v}_m \right) - \left( \frac{\partial}{\partial x} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial y} \right) + \frac{\partial}{\partial z} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial z} \right) \right) + \dot{r}_A$$

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

$$\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v}_m \cdot \nabla \omega_A + \omega_A \nabla \cdot \underline{v}_m \right) - \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho D_{AB} \frac{\partial \omega_A}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial z} \right) \right) + \dot{r}_A$$

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

$$\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v}_m \cdot \nabla \omega_A + \omega_A \nabla \cdot \underline{v}_m \right) - \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho D_{AB} \frac{\partial \omega_A}{\partial r} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \rho D_{AB} \frac{\partial \omega_A}{\partial \theta} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \left( \rho D_{AB} \frac{\partial \omega_A}{\partial \phi} \right) \right) + \dot{r}_A$$

**Fick's law of diffusion, Gibbs notation**  $\underline{j}_A = \omega_A \underline{v}_m + \underline{j}_A^*$

**Fick's law of diffusion, Cartesian coordinates**  $\begin{pmatrix} j_{Ax} \\ j_{Ay} \\ j_{Az} \end{pmatrix} = \omega_A \begin{pmatrix} v_{mx} \\ v_{my} \\ v_{mz} \end{pmatrix} + \begin{pmatrix} j_{Ax}^* \\ j_{Ay}^* \\ j_{Az}^* \end{pmatrix}$

**Fick's law of diffusion, cylindrical coordinates**  $\begin{pmatrix} j_{Ar} \\ j_{A\theta} \\ j_{Az} \end{pmatrix} = \omega_A \begin{pmatrix} v_{mr} \\ v_{m\theta} \\ v_{mz} \end{pmatrix} + \begin{pmatrix} j_{Ar}^* \\ j_{A\theta}^* \\ j_{Az}^* \end{pmatrix}$

**Fick's law of diffusion, spherical coordinates**  $\begin{pmatrix} j_{Ar} \\ j_{A\theta} \\ j_{A\phi} \end{pmatrix} = \omega_A \begin{pmatrix} v_{mr} \\ v_{m\theta} \\ v_{m\phi} \end{pmatrix} + \begin{pmatrix} j_{Ar}^* \\ j_{A\theta}^* \\ j_{A\phi}^* \end{pmatrix}$

## Law of Species Diffusion

### QUESTION:

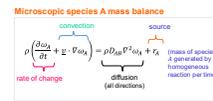
Why so many versions of species A flux?

### 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?

$N_A$  – combined molar flux (includes convection and diffusion)  
 $\dot{M}_A$  – combined mass flux (includes convection and diffusion)  
 $\dot{J}_A$  – mass flux (diffusion only)  
 $\dot{J}_A^*$  – molar flux (diffusion only)



#### Written relative to what velocity?

$N_A$  – relative to stationary coordinates  
 $\dot{M}_A$  – relative to stationary coordinates  
 $\dot{J}_A$  – relative to the mass average velocity  $\mathbf{v}$   
 $\dot{J}_A^*$  – relative to the molar average velocity  $\mathbf{v}^*$

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.

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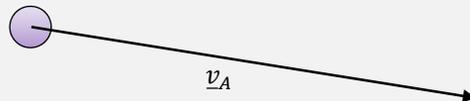
## “Flux” of Species A in a Mixture with Species B

### 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,  $\mathbf{v}_A$  is the **average velocity** (speed and direction) of the A molecules:

$$\mathbf{v}_A = \frac{1}{n_T} \sum_{i=1}^{n_T} \mathbf{v}_{A,i} \quad (\text{a regular average})$$



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**

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“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**

$\underline{v}_A$

**velocity of molecules of species *A*, on average**

(in a region of space)

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“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**

$\underline{v}_A$

**velocity of molecules of species *A*, on average**

(in a region of space)

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

**Is this  $\underline{v}$ ?**

**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:  $\rho \left( \frac{\partial \underline{v}}{\partial t} + \underline{v} \cdot \nabla \underline{v} \right) = -\nabla p + \underline{f} + \rho \underline{g}$  **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:  $\rho \left( \frac{\partial E}{\partial t} + \underline{v} \cdot \nabla E \right) = -\nabla \cdot \underline{q} + S_e$  **general conduction**

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

(incompressible fluid, constant pressure, neglect  $E_v$ , viscous dissipation)

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"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?**

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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      (continuum is divided into mass "particles")

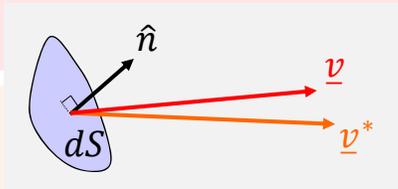
$$\rho d\dot{V} = \rho(\hat{n} \cdot \underline{v}) dS$$

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

**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:  $v^*$  = the molar average velocity      © Faith A. Morrison, Michigan Tech U. <sup>33</sup>

"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 and is not the same:

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

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

molar average velocity of individual molecules

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

Sorry about the re-used nomenclature:  $v^*$  = the molar average velocity      © Faith A. Morrison, Michigan Tech U. <sup>34</sup>

**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.

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

"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  $\bar{v}$  is the **mass** average velocity of the **molecular** velocities  $\bar{v}_A$  and  $\bar{v}_B$ .

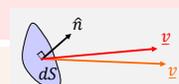
**local mass flow**  $\rho dV = \rho(\hat{n} \cdot \bar{v}) dS$

*mass average velocity of individual molecules*  
 $\bar{v} = \omega_A \bar{v}_A + \omega_B \bar{v}_B$

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

**local molar flow**  $c dV = c(\hat{n} \cdot \bar{v}^*) dS$

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



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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?**

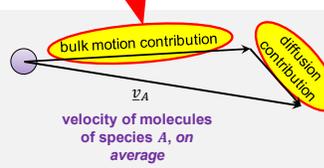
**Two contributions:**

- **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?



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First Approach

“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?**

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.

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First Approach

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

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

**Now, what is this?**

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

**First Approach**

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

bulk motion contribution  $\underline{v}$

diffusion contribution  $(\underline{v}_A - \underline{v})$

$\underline{v}_A$

**Start with mass flux:**

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

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

volumetric flow rate per area in the direction of diffusion

volumetric flow rate per area in the direction of diffusion

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

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

Fick's law in mass terms

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

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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?**

bulk motion contribution  $\underline{v}$

diffusion contribution  $(\underline{v}_A - \underline{v})$

$\underline{v}_A$

**What if I want to use a molar flux?**

Second Approach

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Second Approach

**“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?**

$\underline{v}_A$

**Answer:**  
**This is possible too.**

**What if I want to use a molar flux?**

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  $\neq \underline{v}$**

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

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Second Approach

**“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?**

$\underline{v}_A$

**Answer:**  
**This is possible too.**

**What if I want to use a molar flux?**

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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