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

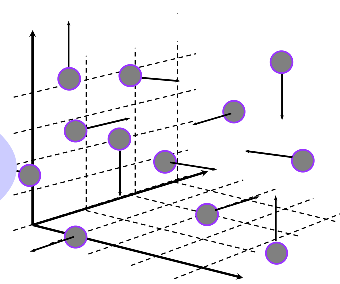
 1

CM3120: Module 3

Module 3 Lecture V

Microscopic Species A Balances

(3 versions)



Professor Faith A. Morrison
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www.chem.mtu.edu/~fmorriso/cm3120/cm3120.html

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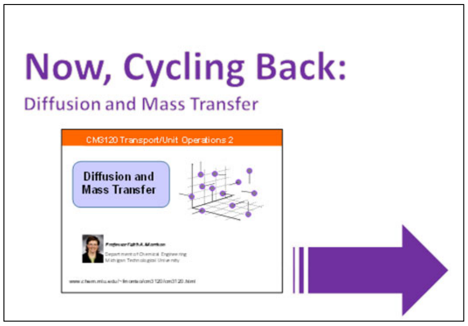
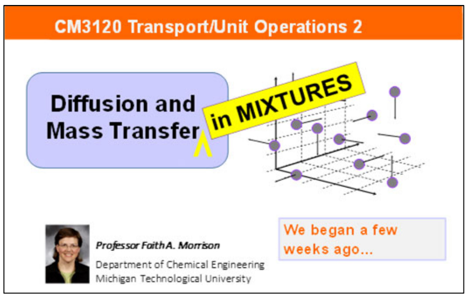




What is the species A mass balance?

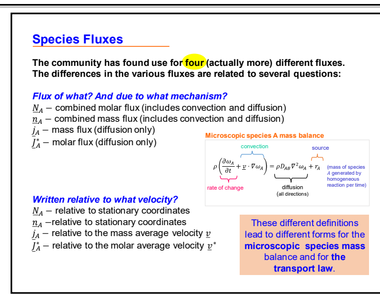
Why are there so many versions?

Last time…

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.

Last time…

The average speed of A molecules in a region of space has a ***bulk motion*** contribution and a ***diffusion*** contribution.

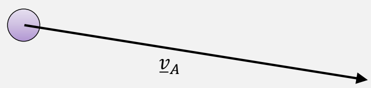
"Flux" of Species A in a Mixture with Species B

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:

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

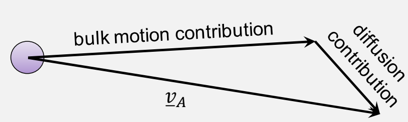
 5

Last time…

These two contributions need not be ***colinear***.

"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**



velocity of molecules of species A, *on average*

(in a region of space)

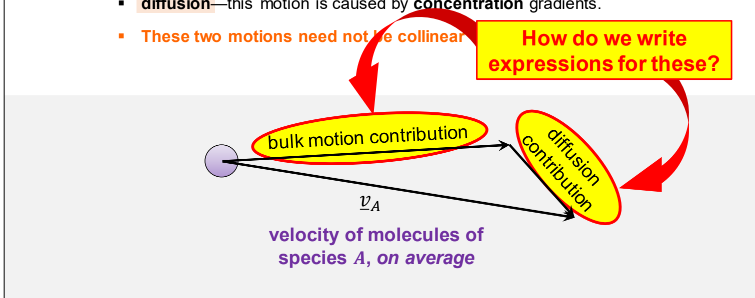
 6

Last time…

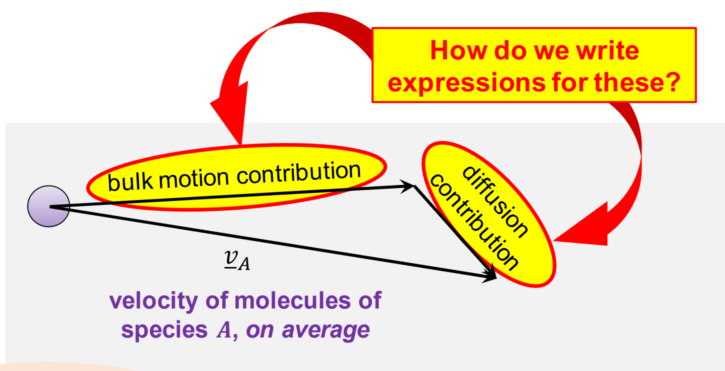
Should we use a **mass average velocity** $\underline{v}$ or a **molar average velocity** $\underline{v}^*$ for the bulk contribution?

"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**



Should we use a **mass average velocity** $\underline{v}$ or a **molar average velocity** $\underline{v}^*$ for the bulk contribution?



Each has advantages and disadvantages.

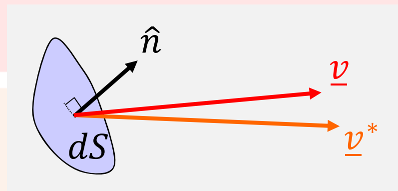
"Flux" of Species A in a Mixture with Species B

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 $\underline{v}_B$

$$\overbrace{\rho\, d\dot{V}}^{\text{local mass flow}} = \rho(\,\hat{n}\cdot \underline{v})\, dS$$

mass average velocity of individual molecules

(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:***

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

molar average velocity of individual molecules

(continuum is divided into molar "particles")

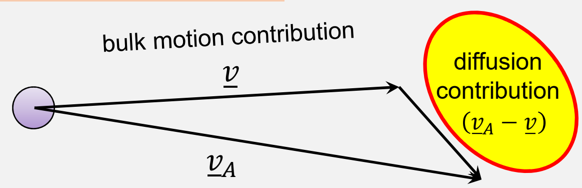
Sorry about the re-used nomenclature: v^* = the molar average velocity

 9

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

First Approach

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



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

Start with mass flux:

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

$$= \underbrace{(\underline{v}_A - \underline{v})}_{\text{volumetric flow rate per area in the direction of diffusion}}\ \rho\, \omega_A$$

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

Fick's law in mass terms

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

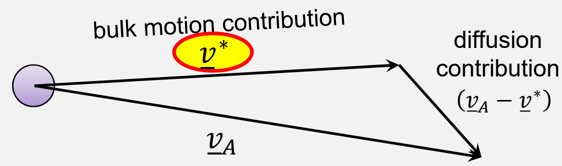
Recall in a pipe: $\frac{\dot{V}}{area} = \langle v \rangle$

 10

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

Second Approach

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



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

Start with molar flux:

$$\text{Molar flux of } A \equiv \frac{moles\ A\ diffusing}{area \cdot time}$$

$$= \underbrace{(\underline{v}_A - \underline{v}^*)}_{\text{volumetric flow rate per area in the direction of diffusion}}\ c\ x_A \qquad \equiv \underline{J}_A^* = ?$$

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

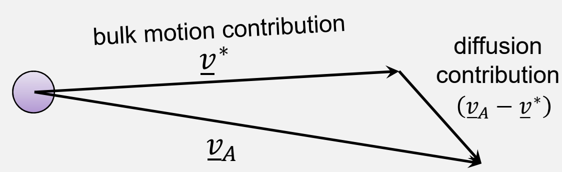
Recall in a pipe: $\frac{\dot{V}}{area} = \langle v \rangle$

11

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

Second Approach

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



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

Start with molar flux:

$$\text{Molar flux of } A \equiv \frac{moles\ A\ diffusing}{area \cdot time}$$

$$= \underbrace{(\underline{v}_A - \underline{v}^*)}_{\text{volumetric flow rate per area in the direction of diffusion}}\ c\ x_A \qquad \equiv \underline{J}_A^* = ?$$

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

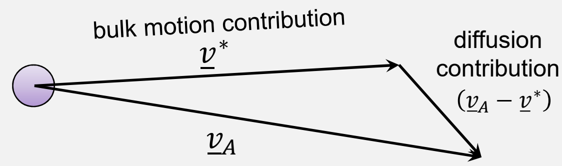
What is Fick's law in terms of this molar flux?

12

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

Second Approach

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



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

Start with molar flux:

$$\text{Molar flux of } A \equiv \frac{moles\ A\ diffusing}{area \cdot time}$$

$$= (\underline{v}_A - \underline{v}^*)\, c\, x_A \quad \equiv \underline{J}_A^* = ?$$

What is Fick’s law in terms of this molar flux?

To answer, we start with the other version of Fick’s law and do the math…

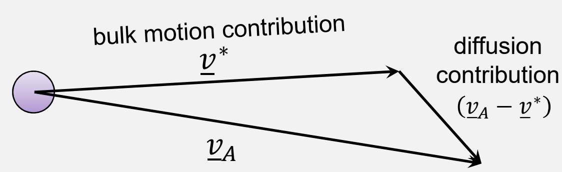
https://pages.mtu.edu/~fmorriso/cm3120/DeriveFicksLawWithMolarUnits2021.pdf

13

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

Second Approach

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



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

Start with molar flux:

$$\text{Molar flux of } A \equiv \frac{moles\ A\ diffusing}{area \cdot time}$$

$$= (\underline{v}_A - \underline{v}^*)\, c\, x_A$$

Result:

$$\boxed{\equiv \underline{J}_A^* = -cD_{AB} \nabla x_A}$$

Fick’s law in molar terms

volumetric flow rate per area in the direction of diffusion

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

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

14

Summary:

Possible fluxes so far:

$\underline{J}_A^* = (\underline{v}_A - \underline{v}^*)\, cx_A$ = **molar** flux relative to **molar** average velocity $\underline{v}^*$
$\underline{j}_A = (\underline{v}_A - \underline{v})\, \rho\omega_A$ = **mass** flux relative to **mass** average velocity $\underline{v}$

Combined fluxes are also in use:

$\underline{N}_A = cx_A \underline{v}_A$ = combined molar flux relative to stationary coordinates
$\underline{n}_A = \rho\omega_A \underline{v}_A$ = combined mass flux relative to stationary coordinates

Mass

$$\underline{j}_A = \rho\omega_A(\underline{v}_A - \underline{v}) = \rho\omega_A\underline{v}_A - \rho\omega_A\underline{v}$$
$$\underline{n}_A \equiv \underline{j}_A + \rho\omega_A\underline{v} = \rho\omega_A\underline{v}_A$$

Moles

$$\underline{J}_A^* = cx_A(\underline{v}_A - \underline{v}^*) = cx_A\underline{v}_A - cx_A\underline{v}^*$$
$$\underline{N}_A \equiv \underline{J}_A^* + cx_A\underline{v}^* = cx_A\underline{v}_A$$

All our previous flux expressions (momentum and energy) have been with respect to stationary coordinates. In diffusion, this points to the use of combined fluxes.

Various forms of Fick's Law

Summary:

Possible fluxes so far:

$\underline{J}_A^* = (\underline{v}_A - \underline{v}^*)\, cx_A$ =
$\underline{j}_A = (\underline{v}_A - \underline{v})\, \rho\omega_A$ =

Also, it can be hard/impossible/*pointless* to separate *convection* and *diffusion*

Combined fluxes are also in use:

$\underline{N}_A = cx_A \underline{v}_A$ = combined molar flux relative to stationary coordinates
$\underline{n}_A = \rho\omega_A \underline{v}_A$ = combined mass flux relative to stationary coordinates

Mass

$$\underline{j}_A = \rho\omega_A(\underline{v}_A - \underline{v}) = \rho\omega_A\underline{v}_A - \rho\omega_A\underline{v}$$
$$\underline{n}_A \equiv \underline{j}_A + \rho\omega_A\underline{v} = \rho\omega_A\underline{v}_A$$

Moles

$$\underline{J}_A^* = cx_A(\underline{v}_A - \underline{v}^*) = cx_A\underline{v}_A - cx_A\underline{v}^*$$
$$\underline{N}_A \equiv \underline{J}_A^* + cx_A\underline{v}^* = cx_A\underline{v}_A$$

All our previous flux expressions (momentum and energy) have been with respect to stationary coordinates. In diffusion, this points to the use of combined fluxes.

Various forms of Fick's Law

When do we use what?

Four possible fluxes:

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

The fluxes $\underline{J}_A^*$ **and** $\underline{j}_A$ are used to describe the mass transfer in diffusion cells used for measuring the diffusion coefficient.

The fluxes relative to coordinates fixed in space $\underline{n}_A$ **and** $\underline{N}_A$ are often used to describe engineering operations within process equipment.

WRF p440

17

Various forms of Fick's Law

When do we use what?

Four possible fluxes:

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

The mass fluxes $\underline{n}_A$ **and** $\underline{j}_A$ are used when the Navier-Stokes equations are also required to describe the process (same $\underline{v}$), e.g. dimensional analysis.

Since chemical reactions are described in terms of moles of the participating reactants, the molar fluxes $\underline{J}_A^*$ **and** $\underline{N}_A$ are used to describe mass-transfer operations in which homogeneous chemical reactions are involved ($R_A \neq 0$)

WRF p440

18

When do we use what?

Four possible fluxes:

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

1. The mass fluxes **$\underline{n}_A$ and $\underline{j}_A$** are used when the Navier-Stokes equations are also required to describe the process since they use $\underline{v}$.
2. Since chemical reactions are described in terms of moles of the participating reactants, the molar fluxes **$\underline{J}_A^*$ and $\underline{N}_A$** are used to describe mass-transfer operations in which homogeneous chemical reactions are involved.
3. The fluxes relative to coordinates fixed in space **$\underline{n}_A$ and $\underline{N}_A$** are often used to describe engineering operations within process equipment
4. The fluxes **$\underline{J}_A^*$ and $\underline{j}_A$** are used to describe the mass transfer in diffusion cells used for measuring the diffusion coefficient

WRF p440

What now?

Four Fluxes.
Four Microscopic Species A Balances.

Various forms of Fick's Law

What now?

Four Fluxes.

~~Four~~ Microscopic Species A Balances.
Three

(We do not often use the combined mass flux version, $\underline{n}_A$).

Next?
***Derive* (indicate derivation of) Microscopic Species A Balances.**

21

Various forms of the Microscopic Species A Mass Balance

Derivation of Microscopic Species A Mass balance (Quick tour)

Mass Balance: Body versus Control Volume

Law of Mass Conservation: (on a **body**)

$$\boxed{\frac{dM_B}{dt} = 0}$$

Law of Mass Conservation: (on a **control volume**)

$$\frac{dM_{CV}}{dt} = \underbrace{\iint_{CS} -(\hat{n} \cdot \underline{v})\rho dS}_{\text{the } usual \text{ convective term: net mass convected } in}$$

WRF, p467

22

Various forms of the Microscopic Species A Mass Balance

Species A Mass Balance:

Law of **Species A** Mass Conservation:
(**on a body,** with homogeneous reaction)

$$\boxed{\frac{dM_{A,B}}{dt} = r_A}$$

Law of **Species A** Mass Conservation:
(**on a control volume,** with homogeneous reaction)

$$\frac{dM_{A,CV}}{dt} = \underbrace{\iint_{CS} -(\hat{n} \cdot \underline{v})\rho dS}_{} + r_A$$

the *usual* convective term:
net mass *in* from all sources

bulk flow PLUS mass of species A that ***diffuses*** into CV

Various forms of the Microscopic Species A Mass Balance

Species A Mass Balance:

Law of **Species A** Mass Conservation:
(**on a body,** with homogeneous reaction)

$$\boxed{\frac{dM_{A,B}}{dt} = r_A}$$

Law of **Species A** Mass Conservation:
(**on a control volume,** with homogeneous reaction)

$$\frac{dM_{A,CV}}{dt} = \underbrace{\iint_{CS} -(\hat{n} \cdot \underline{v})\rho dS}_{} + r_A$$

Diffusion is the study of *species* *motion* in *mixtures*.

the *usual* convective term:
net mass *in* from all sources

bulk flow PLUS mass of species A that ***diffuses*** into CV

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Various forms of the Microscopic Species A Mass Balance

Species A Mass Balance, on a CV:

Law of Species Mass Conservation: (**on a control volume,** with homogeneous reaction)

$$\frac{dM_{A,CV}}{dt} = \iint_{CS} -(\hat{n} \cdot \underline{v})dS + r_A$$

…

Law of Species Mass Conservation: (**microscopic control volume,** with homogeneous reaction)

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

Various forms of the Microscopic Species A Mass Balance

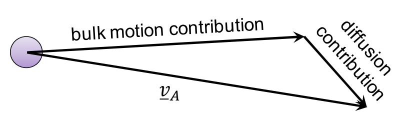
Microscopic Species A Mass Balance, on a CV:

Law of Species Mass Conservation: (**microscopic control volume,** with homogeneous reaction)

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

Diffusion: $\underline{j}_A [=] \dfrac{mass\ A}{area \cdot time}$

$\underline{j}_A \equiv$ mass flux of species A relative to a mixture's mass average velocity $\underline{v}$



Various forms of the Microscopic Species A Mass Balance

Microscopic Species A Mass Balance, on a CV:

Law of Species Mass Conservation: (**microscopic control volume,** with homogeneous reaction)

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

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 ($\underline{j}_A$) appears (p. 1), and the more usual case (p. 2), where the diffusion coefficient is constant and Fick's law has been incorporated.

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In terms of mass flux, $\underline{j}_A$

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

$$\rho\left(\frac{\partial \omega_A}{\partial t} + v_r\frac{\partial \omega_A}{\partial r} + \frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta} + \frac{v_\phi}{r\sin\theta}\frac{\partial \omega_A}{\partial \phi}\right) = -\left(\frac{1}{r^2}\frac{\partial (r^2 j_{A,r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (j_{A,\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial j_{A,\phi}}{\partial \phi}\right) + r_A$$

FRONT

27

Various forms of the Microscopic Species A Mass Balance

What is this mass conservation equation in terms of molar quantities?

Law of Species Mass Conservation: (**microscopic control volume,** with homogeneous reaction)

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

Molar flux of $A \equiv \dfrac{moles\ A\ diffusing}{area\cdot time}$

$$= (\underline{v}_A - \underline{v}^*)\, c\, x_A \equiv \underline{J}_A^*$$

To answer, we start with the other version of Fick's law and do the math…

https://pages.mtu.edu/~fmorriso/cm3120/DeriveFicksLawWithMolarUnits2021.pdf

28

Various forms of the Microscopic Species A Mass Balance

What is this mass conservation equation in terms of molar quantities?

Law of Species Mass Conservation: (**microscopic control volume,** with homogeneous reaction)

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

In terms of molar flux and molar concentrations

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

And, likewise, we can reformulate in terms of combined molar flux.

Various forms of the Microscopic Species A Mass Balance

Microscopic species A mass balance—Six 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

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

Various forms of the Microscopic Species A Mass Balance

Microscopic species A mass balance—~~Six~~ 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

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

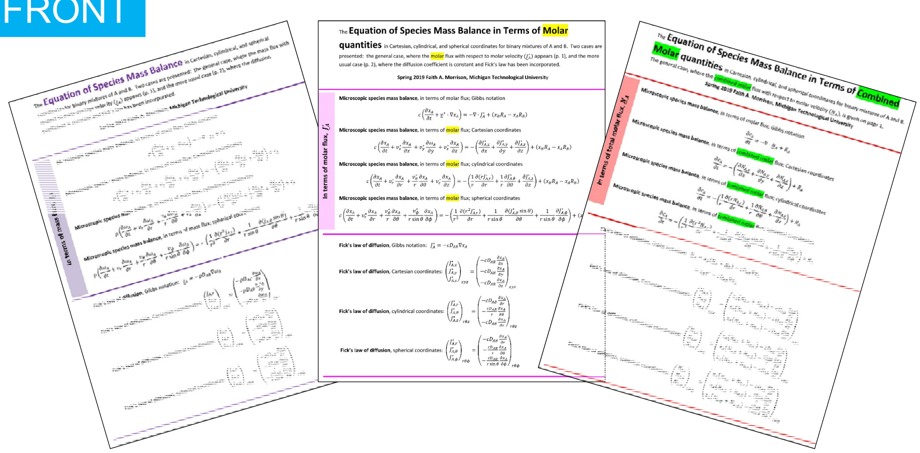
(The combined molar flux version cannot easily have Fick's law substituted in.)

31

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



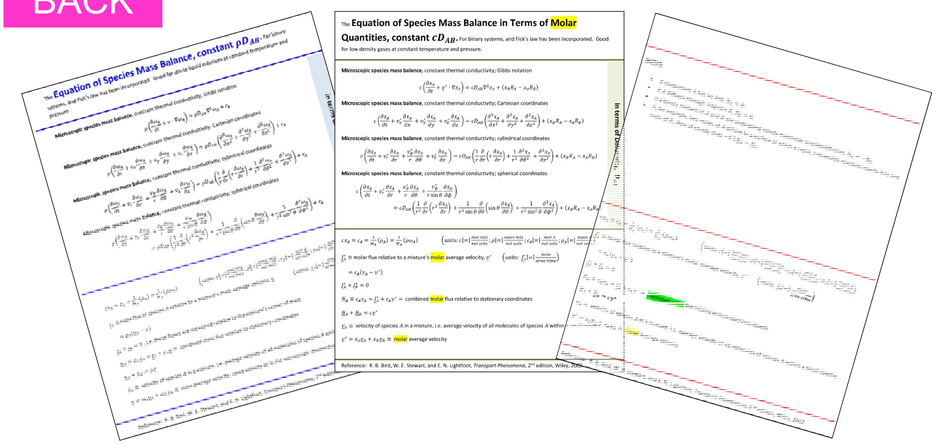
pages.mtu.edu/~fmorriso/cm3120/Homeworks_Readings.html

32

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

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

BACK



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33

SUMMARY: 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**

$\underline{N}_A + \underline{N}_B = c \underline{v}^*$

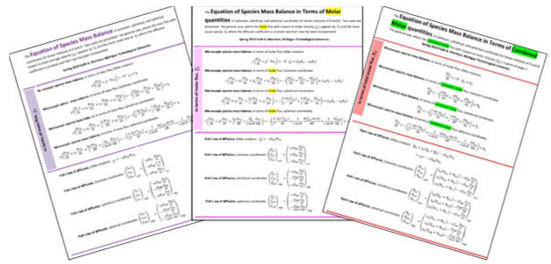
$\underline{v}_A \equiv$ velocity of species A in a mixture, i.e. average velocity of all molecules of species A within a small volume

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

34

Let's put this to use



Various forms of the Microscopic Species A Mass Balance

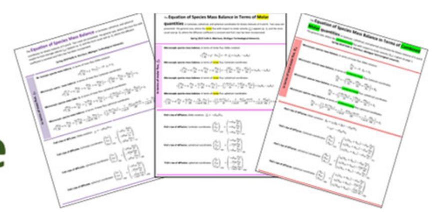
Microscopic species A mass balance—~~Six~~ Five forms

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

35

1D Steady Diffusion

Let's put this to use



1D Steady Diffusion Problems

1. 1D simple rectangular mass transfer (evaporating tank, **Ex 1**) QUICK START
2. 1D radial mass transfer (evaporating droplet, **Ex 2**) QUICK START
3. More…

36