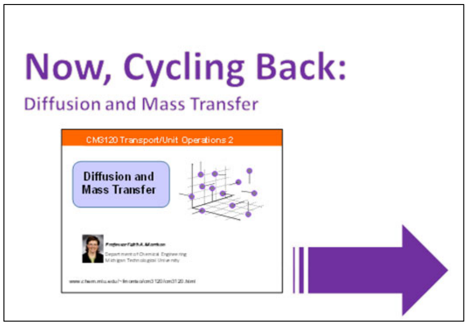
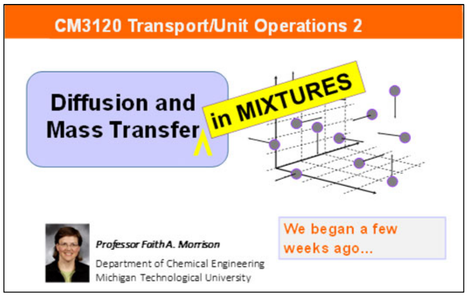


Now, Cycling Back:

Diffusion and Mass Transfer

CM3120 Transport/Unit Operations 2

Diffusion and Mass Transfer



CM3120 Transport/Unit Operations 2

Diffusion and Mass Transfer in MIXTURES

Professor Faith A. Morrison

Department of Chemical Engineering
Michigan Technological University

We began a few weeks ago…

What is the species A mass balance?

Why are there so many versions?

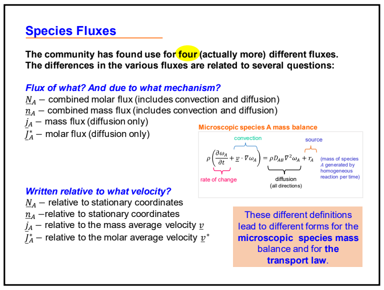
Continuing…

Last time…

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

$$\rho\left(\underbrace{\frac{\partial\omega_A}{\partial t}}_{\text{rate of change}}+\overbrace{\underline{v}\cdot\nabla\omega_A}^{\text{convection}}\right)=\underbrace{\rho D_{AB}\nabla^2\omega_A}_{\substack{\text{diffusion}\\ \text{(all directions)}}}+\overbrace{r_A}^{\text{source}}$$

(mass of species *A* generated by homogeneous reaction per time)

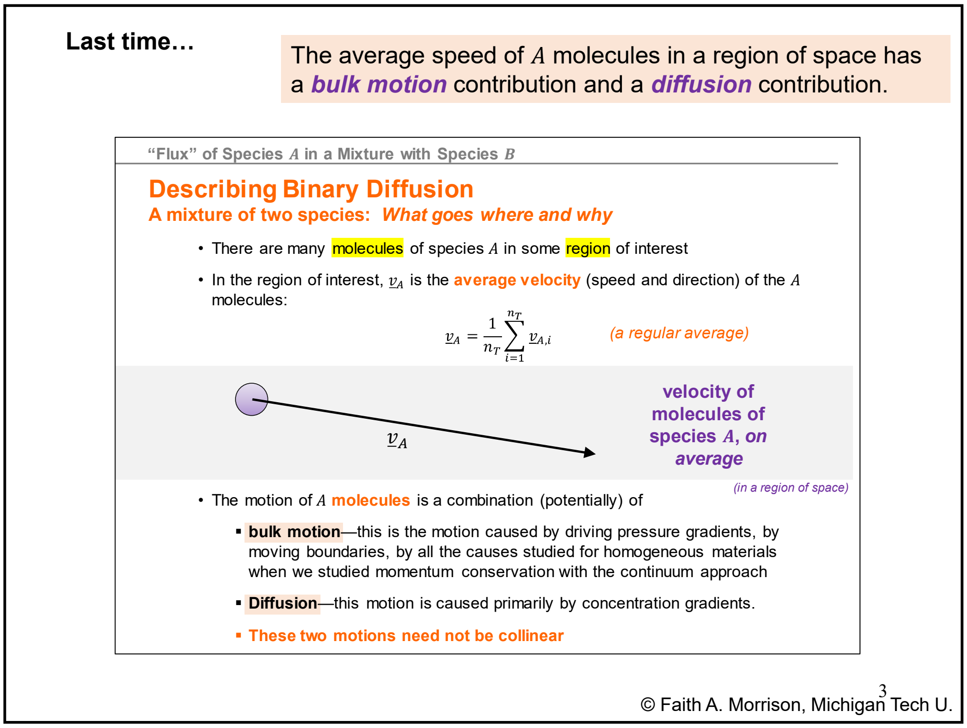
Written relative to what velocity?

$\underline{N}_A$ – 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.



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:

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

$\underline{v}_A$

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**

3

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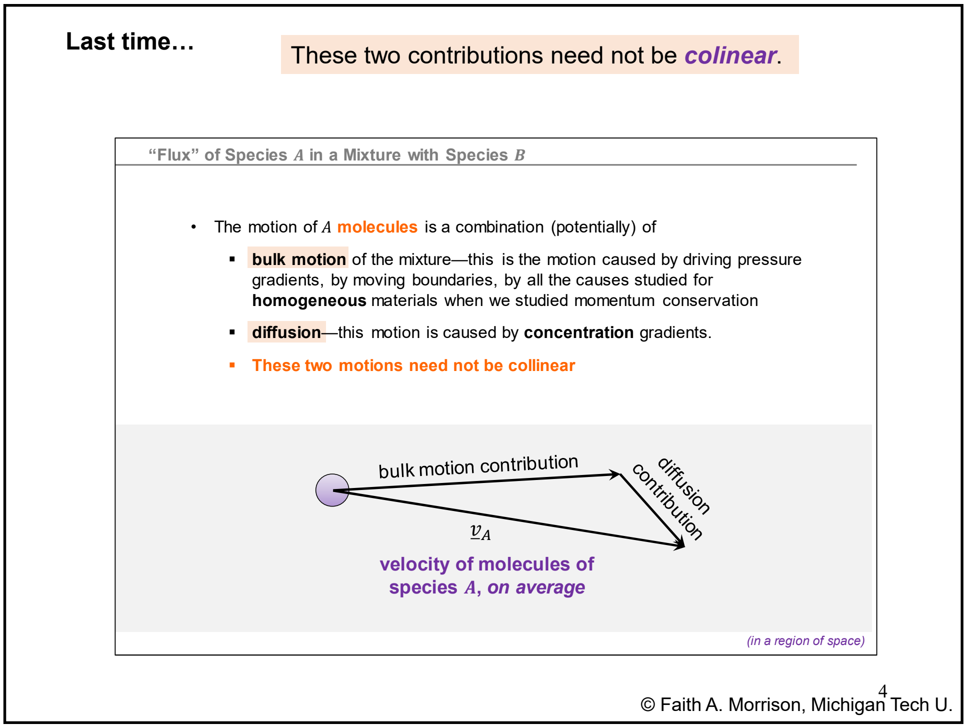

Last time…

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**

bulk motion contribution

diffusion contribution

$\underline{v}_A$

velocity of molecules of species A, *on average*

(in a region of space)

4

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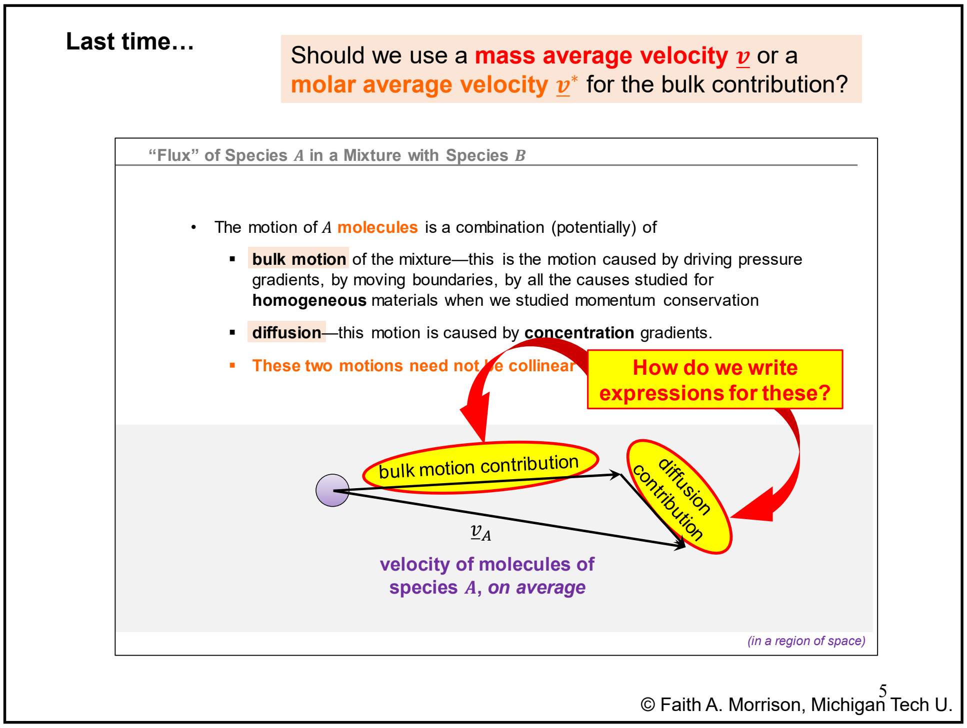

Last time…

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**

How do we write expressions for these?

bulk motion contribution

diffusion contribution

$\underline{v}_A$

velocity of molecules of species A, *on average*

(in a region of space)

5

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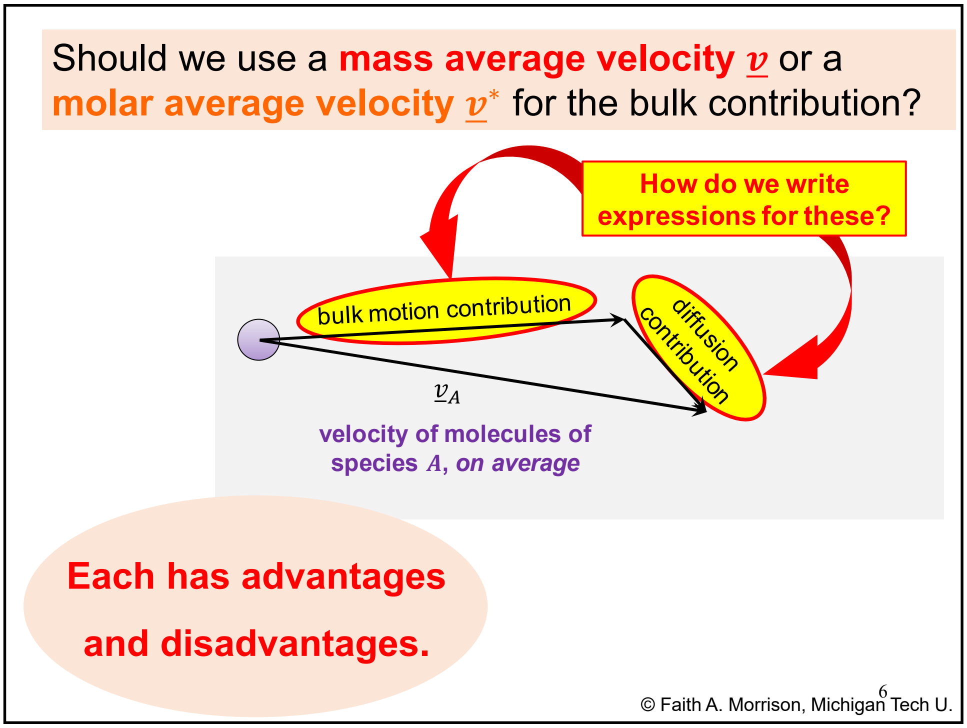

Should we use a **mass average velocity $\underline{v}$** or a **molar average velocity $\underline{v}^*$** for the bulk contribution?

How do we write expressions for these?

bulk motion contribution

diffusion contribution

$\underline{v}_A$

velocity of molecules of species A, *on average*

Each has advantages and disadvantages.

6

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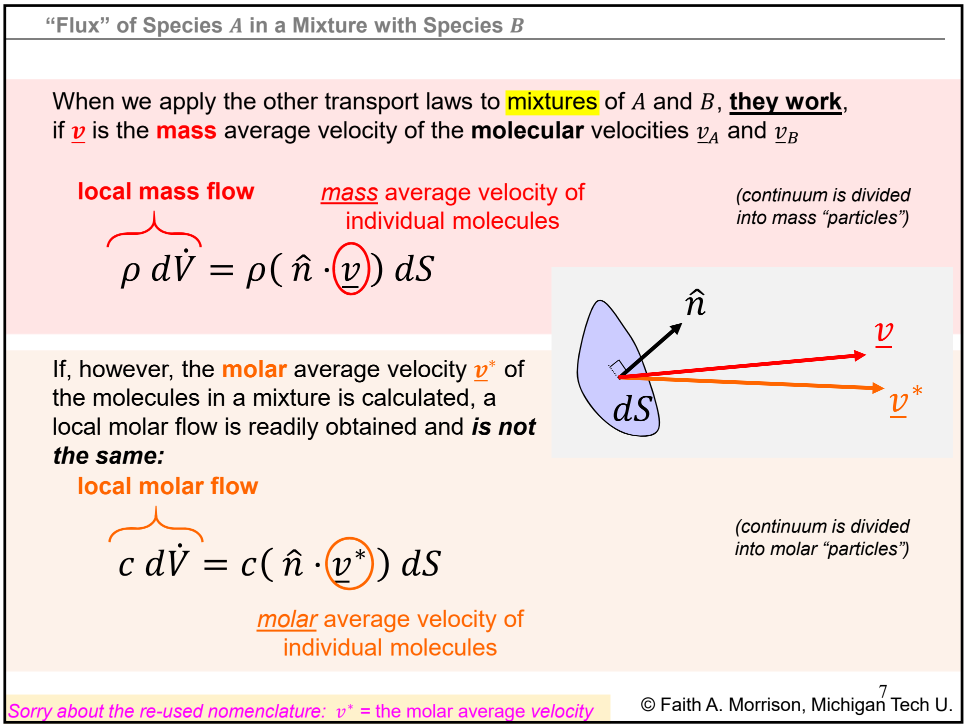

“Flux” of Species A in a Mixture with Species B

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

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

(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

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

(continuum is divided into molar “particles”)

molar average velocity of individual molecules

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

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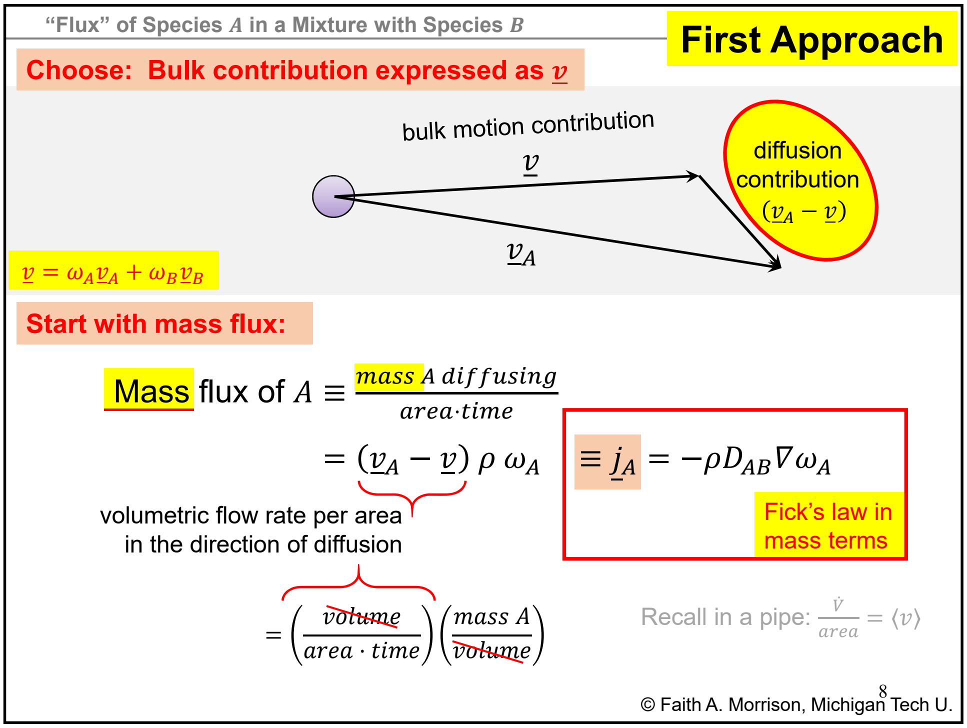

“Flux” of Species A in a Mixture with Species B

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:

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

$$= \underbrace{(\underline{v}_A - \underline{v})}_{\text{volumetric flow rate per area in the direction of diffusion}}\, \rho\, \omega_A \;\; \boxed{\equiv \underline{j}_A = -\rho D_{AB} \nabla \omega_A}$$

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

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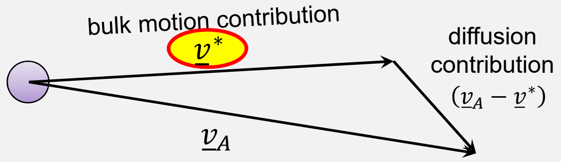
“Flux” of Species A in a Mixture with Species B

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:

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

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

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

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

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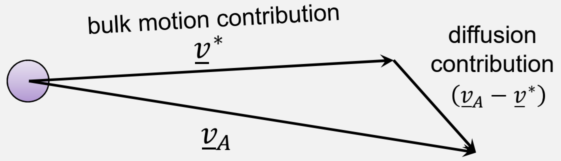
“Flux” of Species A in a Mixture with Species B

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:

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

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

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

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

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

10

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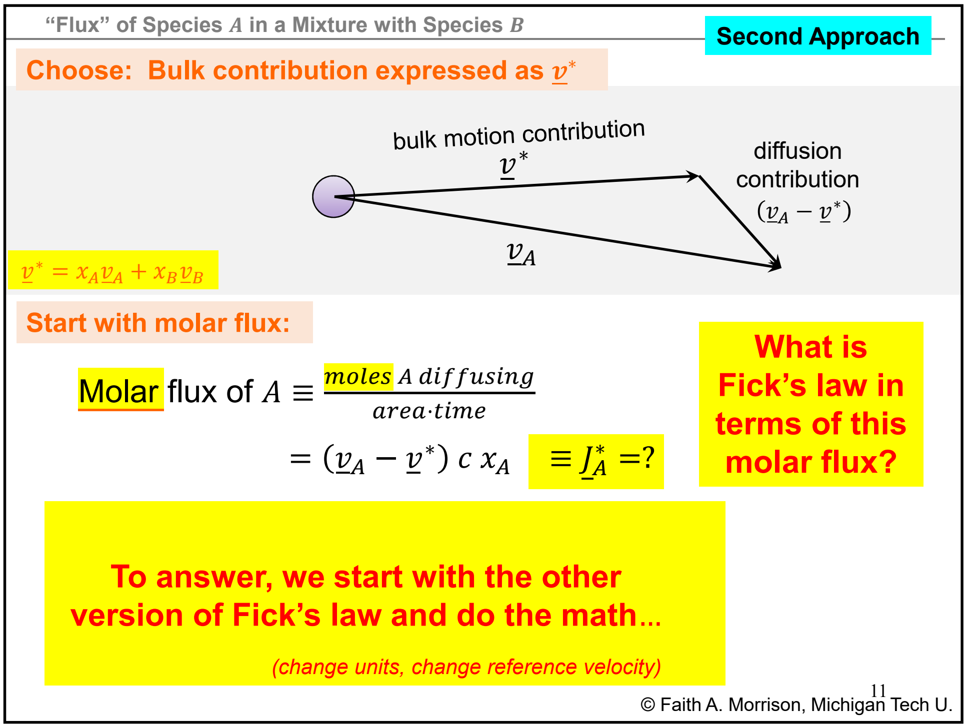


"Flux" of Species A in a Mixture with Species B

Second Approach

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

bulk motion contribution $\underline{v}^*$

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

$\underline{v}_A$

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

Start with molar flux:

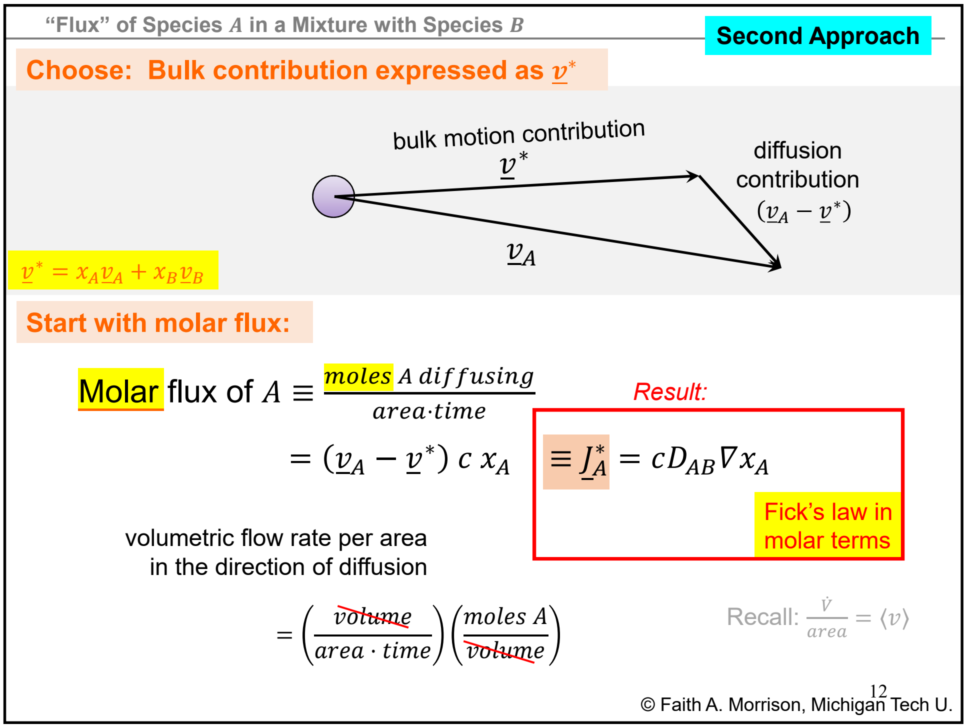
$$\text{Molar flux of } A \equiv \frac{moles\ A\ diffusing}{area \cdot time}$$

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

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…

(change units, change reference velocity)



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

Second Approach

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

bulk motion contribution $\underline{v}^*$

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

$\underline{v}_A$

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

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

Summary:

Possible fluxes so far:

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

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

Mass

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

Moles

$$\begin{aligned} \underline{J}_A^* &= c x_A(\underline{v}_A - \underline{v}^*) \\ &= c x_A\underline{v}_A - c x_A\underline{v}^* \\ \underline{N}_A \equiv \underline{J}_A^* + c x_A\underline{v}^* &= c x_A\underline{v}_A \end{aligned}$$

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.

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

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

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

Various forms of Fick's Law

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.

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**)

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

the *usual* convective term:
net mass convected *in*

WRF, p467

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)

$$\frac{dM_{A,CV}}{dt} = \underbrace{\iint_{CS} -(\hat{n} \cdot \underline{v})\rho dS}_{\text{the \textit{usual} convective term: net mass \textit{in} from all sources}} + r_A$$

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)

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

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

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

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

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)

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

…

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

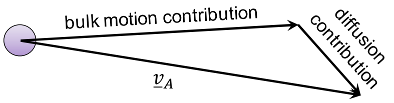
Microscopic Species A Mass Balance, on a CV:

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

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

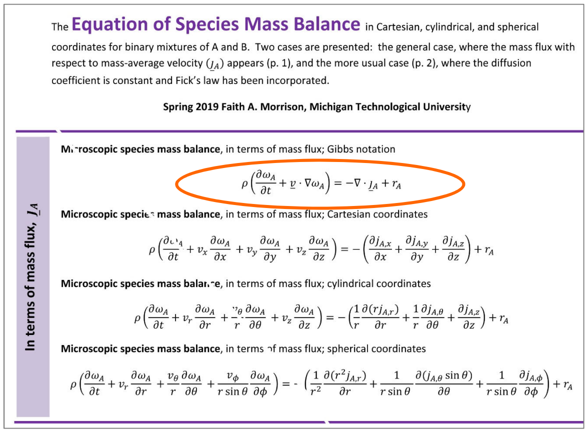


Various forms of the Microscopic Species A Mass Balance

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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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

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

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

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

FRONT

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 $A \equiv \frac{moles\ A\ diffusing}{area\cdot time}$

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

To answer, we (*change* units, *convert* ω_A to x_A, *change* reference velocity) and do the math…

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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

$$c\left(\frac{\partial x_A}{\partial t}+\underline{v}^*\cdot\nabla x_A\right)=-\nabla\cdot\underline{J}_A^*+(x_BR_A-x_AR_B)$$

$$=cD_{AB}\nabla^2x_A+(x_BR_A-x_AR_B)$$

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

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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

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

$$= c D_{AB} \nabla^2 x_A + (x_B R_A - x_A R_B)$$

In terms of combined molar flux and molar concentrations

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

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

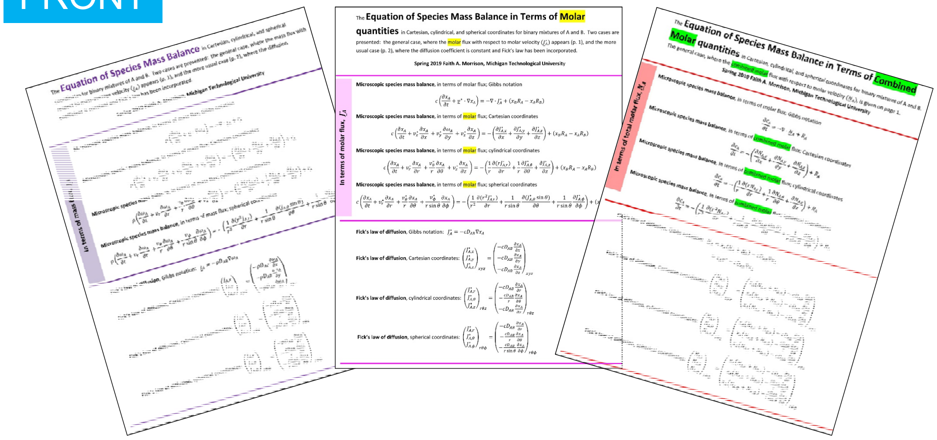
$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

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

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

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

FRONT



The **Equation of Species Mass Balance** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B.

The **Equation of Species Mass Balance in Terms of Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. Two cases are presented: the general case, where the molar flux with respect to molar 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.

Spring 2019 Faith A. Morrison, Michigan Technological University

In terms of molar flux, $\underline{J}_A^*$

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

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

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

$$c\left(\frac{\partial x_A}{\partial t} + v_x^* \frac{\partial x_A}{\partial x} + v_y^* \frac{\partial \omega_A}{\partial y} + v_z^* \frac{\partial x_A}{\partial z}\right) = -\left(\frac{\partial J_{A,x}^*}{\partial x} + \frac{\partial J_{A,y}^*}{\partial y} + \frac{\partial J_{A,z}^*}{\partial z}\right) + (x_B R_A - x_A R_B)$$

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

$$c\left(\frac{\partial x_A}{\partial t} + v_r^* \frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + v_z^* \frac{\partial x_A}{\partial z}\right) = -\left(\frac{1}{r}\frac{\partial (r J_{A,r}^*)}{\partial r} + \frac{1}{r}\frac{\partial J_{A,\theta}^*}{\partial \theta} + \frac{\partial J_{A,z}^*}{\partial z}\right) + (x_B R_A - x_A R_B)$$

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

$$c\left(\frac{\partial x_A}{\partial t} + v_r^* \frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + \frac{v_\phi^*}{r\sin\theta}\frac{\partial x_A}{\partial \phi}\right) = -\left(\frac{1}{r^2}\frac{\partial (r^2 J_{A,r}^*)}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (J_{A,\theta}^* \sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial J_{A,\phi}^*}{\partial \phi}\right) + (x$$

Fick's law of diffusion, Gibbs notation: $\underline{J}_A^* = -cD_{AB}\nabla x_A$

Fick's law of diffusion, Cartesian coordinates: $\begin{pmatrix} J_{A,x}^* \\ J_{A,y}^* \\ J_{A,z}^* \end{pmatrix}_{xyz} = \begin{pmatrix} -cD_{AB}\frac{\partial x_A}{\partial x} \\ -cD_{AB}\frac{\partial x_A}{\partial y} \\ -cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$

Fick's law of diffusion, cylindrical coordinates: $\begin{pmatrix} J_{A,r}^* \\ J_{A,\theta}^* \\ J_{A,z}^* \end{pmatrix}_{r\theta z} = \begin{pmatrix} -cD_{AB}\frac{\partial x_A}{\partial r} \\ -\frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ -cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$

Fick's law of diffusion, spherical coordinates: $\begin{pmatrix} J_{A,r}^* \\ J_{A,\theta}^* \\ J_{A,\phi}^* \end{pmatrix}_{r\theta \phi} = \begin{pmatrix} -cD_{AB}\frac{\partial x_A}{\partial r} \\ -\frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ -\frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta \phi}$

The **Equation of Species Mass Balance in Terms of Combined Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B.

In terms of total molar flux, $\underline{N}_A$

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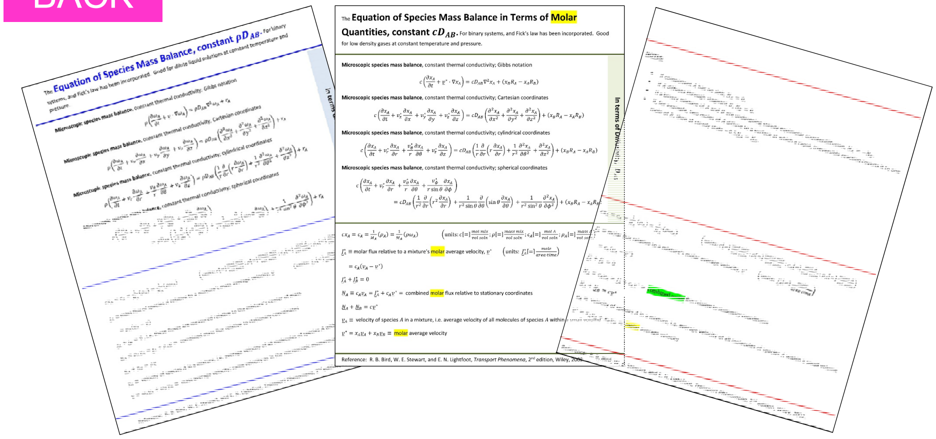
Various forms of Fick's Law (and the species mass balances that employ them)

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

BACK



The **Equation of Species Mass Balance, constant ρD_{AB}.** For binary systems, and Fick's law has been incorporated.

The **Equation of Species Mass Balance in Terms of Molar Quantities, constant cD_{AB}.** For binary systems, and Fick's law has been incorporated. Good for low density gases at constant temperature and pressure.

Microscopic species mass balance, constant thermal conductivity; Gibbs notation

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

Microscopic species mass balance, constant thermal conductivity; Cartesian coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_x^* \frac{\partial x_A}{\partial x} + v_y^* \frac{\partial x_A}{\partial y} + v_z^* \frac{\partial x_A}{\partial z}\right) = cD_{AB}\left(\frac{\partial^2 x_A}{\partial x^2} + \frac{\partial^2 x_A}{\partial y^2} + \frac{\partial^2 x_A}{\partial z^2}\right) + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; cylindrical coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_r^* \frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + v_z^* \frac{\partial x_A}{\partial z}\right) = cD_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial x_A}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 x_A}{\partial \theta^2} + \frac{\partial^2 x_A}{\partial z^2}\right) + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; spherical coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_r^* \frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + \frac{v_\phi^*}{r\sin\theta}\frac{\partial x_A}{\partial \phi}\right)$$
$$= cD_{AB}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial x_A}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial x_A}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 x_A}{\partial \phi^2}\right) + (x_B R_A - x_A R_B)$$

In terms of Diffusivity, D_{AB}

$cx_A = c_A = \frac{1}{M_A}(\rho_A) = \frac{1}{M_A}(\rho\omega_A)$ (units: $c[=]\frac{mol\ mix}{vol\ soln}$; $\rho[=]\frac{mass\ mix}{vol\ soln}$; $c_A[=]\frac{mol\ A}{vol\ soln}$; $\rho_A[=]\frac{mass\ A}{vol\ soln}$)

$\underline{J}_A^* \equiv$ molar flux relative to a mixture's molar average velocity, $\underline{v}^*$ (units: $\underline{J}_A^*[=]\frac{mole}{area\cdot time}$)

$= c_A(\underline{v}_A - \underline{v}^*)$

$\underline{J}_A^* + \underline{J}_B^* = 0$

$\underline{N}_A \equiv c_A\underline{v}_A = \underline{J}_A^* + c_A\underline{v}^* =$ 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

$\underline{v}^* = x_A\underline{v}_A + x_B\underline{v}_B \equiv$ molar average velocity

Reference: R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2nd edition, Wiley, 2002

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SUMMARY: 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

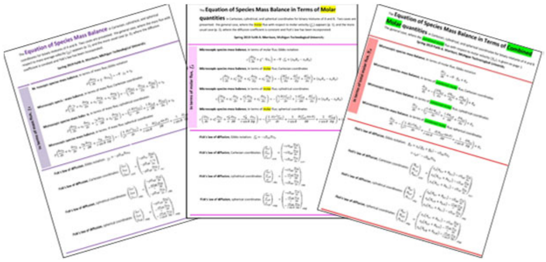
$\underline{n}_A \equiv \rho_A\underline{v}_A = \underline{j}_A + \rho_A\underline{v} =$ **combined mass** flux relative to **stationary coordinates**
$\underline{n}_A + \underline{n}_B = \rho\underline{v}$

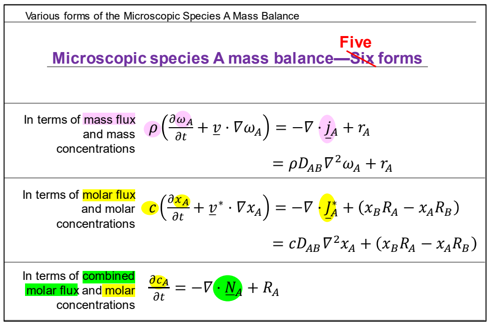
$\underline{J}_A^* \equiv$ **molar** flux relative to a mixture's **molar average velocity**, $\underline{v}^*$
$= c_A(\underline{v}_A - \underline{v}^*)$
$\underline{J}_A^* + \underline{J}_B^* = 0$

$\underline{N}_A \equiv c_A\underline{v}_A = \underline{J}_A^* + c_A\underline{v}^* =$ **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

Let's put this to use

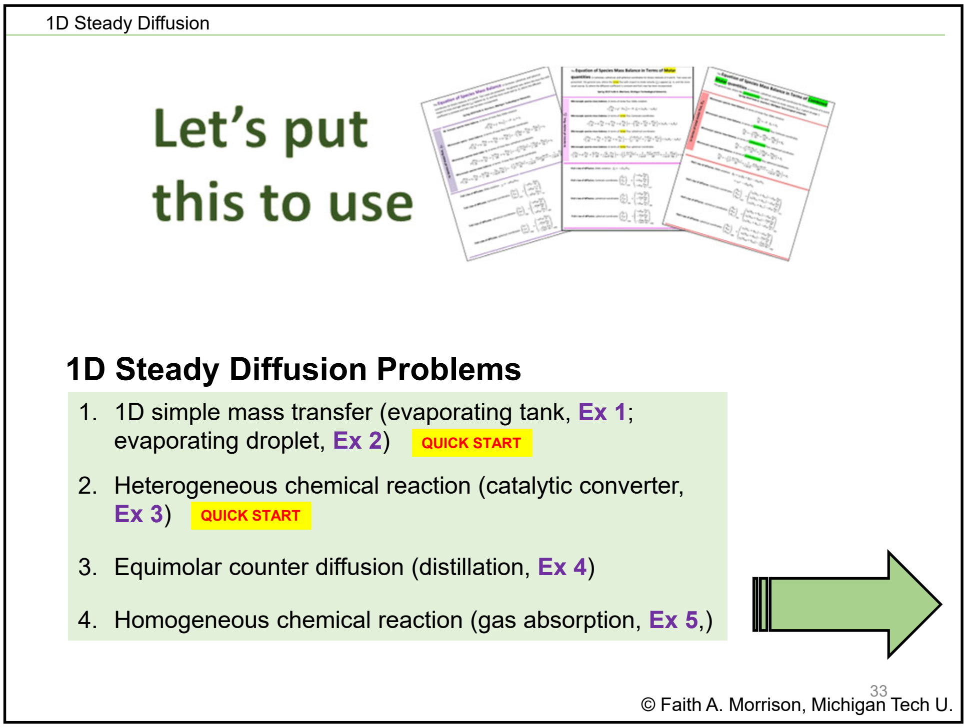




Various forms of the Microscopic Species A Mass Balance

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	$c\left(\frac{\partial x_A}{\partial t} + \underline{v}^*\cdot\nabla x_A\right) = -\nabla\cdot\underline{J}_A^* + (x_BR_A - x_AR_B)$ $= cD_{AB}\nabla^2x_A + (x_BR_A - x_AR_B)$
In terms of combined molar flux and molar concentrations	$\frac{\partial c_A}{\partial t} = -\nabla\cdot\underline{N}_A + R_A$



1D Steady Diffusion

Let’s put this to use

1D Steady Diffusion Problems

1. 1D simple mass transfer (evaporating tank, **Ex 1**; evaporating droplet, **Ex 2**) **QUICK START**
2. Heterogeneous chemical reaction (catalytic converter, **Ex 3**) **QUICK START**
3. Equimolar counter diffusion (distillation, **Ex 4**)
4. Homogeneous chemical reaction (gas absorption, **Ex 5**,)