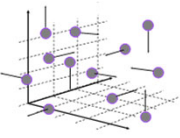



# NEXT: Diffusion and Mass Transfer

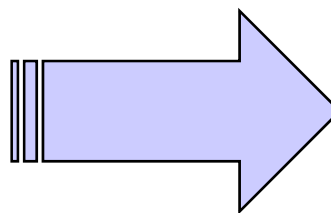
CM3120 Transport/Unit Operations 2

**Diffusion and Mass Transfer**



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

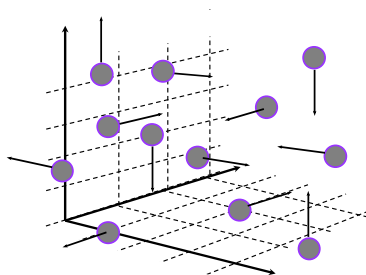
[www.chem.mtu.edu/~fmorriso/cm3120/cm3120.html](http://www.chem.mtu.edu/~fmorriso/cm3120/cm3120.html)



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## CM3120 Transport/Unit Operations 2

### Diffusion and Mass Transfer



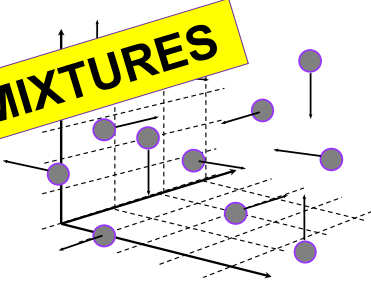
**Professor Faith A. Morrison**  
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[www.chem.mtu.edu/~fmorriso/cm3120/cm3120.html](http://www.chem.mtu.edu/~fmorriso/cm3120/cm3120.html)


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## CM3120 Transport/Unit Operations 2

# Diffusion and Mass Transfer



# in MIXTURES



**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)

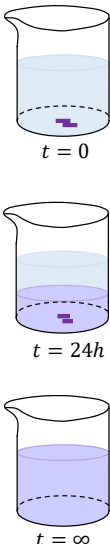
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### Introduction to Diffusion and Mass Transfer in Mixtures

## Diffusion

- Is the mixing process caused by random molecular motion.
- Is part of scientific inquiry (explains how nature works)

**Diffusion/  
mass transfer  
concerns the  
physics of  
mixtures.**



## Mass Transfer

- Encompasses all mass-transfer mechanisms and any issues of mixed physics
- Controls the cost of processes like chemical purification and environmental control
- Is practical (is basic to the engineering of chemical processes)

*References:*  
 E. L. Cussler, *Diffusion: Mass Transfer in Fluid Systems*, 3<sup>rd</sup> edition, Cambridge University Press, 2016.  
 R. B. Bird, W. E. Stewart, E. N. Lightfoot, *Transport Phenomena*, 2<sup>nd</sup> edition, 2002.  
 J. R. Welty, G. L. Rorrer, and D. G. Foster, *Fundamentals of Momentum, Heat and Mass Transfer*, 6<sup>th</sup> edition, 2015.

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Introduction to Diffusion and Mass Transfer in Mixtures

## Diffusion

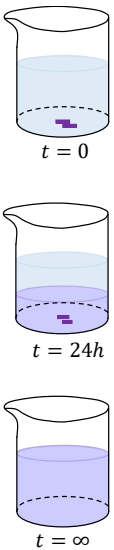
- Is the mixing process caused by random molecular motion (Brownian motion).
- Is part of scientific inquiry (explains how nature works)
- Is slow
- Since it is slow, it acts over short distances

Diffusion progresses at a rate of
 

- $\sim 5\text{cm/min}$  (gases)
- $\sim 0.05\text{cm/min}$  (liquids)
- $\sim 10^{-5}\text{cm/min}$  (solids)

Is the **physics** behind:

- Transport in living cells
- The efficiency of distillation
- The dispersal of pollutants
- Gas absorption
- Fog formed by rain on snow
- The dyeing of wool




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Introduction to Diffusion and Mass Transfer in Mixtures

**Example:** A friend walks into the far end of the room plates of a delicious-smelling warm lunch.  
How did the smell of lunch reach your nostrils?



Diffusion progresses at a rate of

- $\sim 5\text{cm/min}$  (gases)
- $\sim 0.05\text{cm/min}$  (liquids)
- $\sim 10^{-5}\text{cm/min}$  (solids)

# You try.

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## Introduction to Diffusion and Mass Transfer in Mixtures

**Mass Transfer**

- Encompasses all mass-transfer mechanisms: random motion, convection, thermodynamics-driven (specific interaction).
  - Controls the cost of processes like chemical purification and environmental control
  - Is practical (is basic to the engineering of chemical processes)
  - Is also slow
- 
- There is an analogy to heat transfer (but care must be taken not to over emphasize)
  - Dilute mass transfer is emphasized
  - Is the **modeling** behind (for example):
    - ✓ Differential distillation (common) versus staged distillation (less common)
    - ✓ Adsorption
    - ✓ Important applications of mass transfer in biology and medicine
    - ✓ Much more

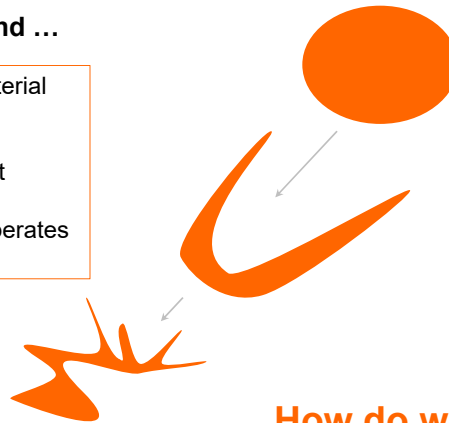
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## Introduction to Diffusion and Mass Transfer in Mixtures

**Mass Transfer****Convection and Diffusion and ...**

- Agitation or stirring moves material over long distances
- Exposing new fluid elements
- Diffusion mixes newly adjacent material
- Because diffusion is slow, it operates only over short distances



**How do we  
model diffusion?**

Reference:  
E. L. Cussler, *Diffusion: Mass Transfer in Fluid  
Systems*, 3<sup>rd</sup> edition, Cambridge University Press, 2016.

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Introduction to Diffusion and Mass Transfer in Mixtures

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## Transport Analogy (flux)

<b><u>Momentum</u></b>	$-\tilde{\tau}_{yz} = -\mu \frac{\partial v_y}{\partial z}$	Newton's Law
<b><u>Heat</u></b>	$\frac{q_z}{A} = -k \frac{\partial T}{\partial z}$	Fourier's Law
<b><u>Species A Mass</u></b> <i>in a mixture with B</i>	$j_{A,z} = -\rho D_{AB} \frac{\partial \omega_A}{\partial z}$	Fick's Law

- ✓ **Momentum** goes down a velocity gradient
- ✓ **Heat** goes down a temperature gradient
- ✓ **Mass of species A** goes down a gradient in concentration of A *in a mixture*

Transport Analogy Reference:  
R. B. Bird, W. E. Stewart, E. N. Lightfoot,  
*Transport Phenomena*, 2<sup>nd</sup> edition, Wiley, 2002.

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Introduction to Diffusion and Mass Transfer in Mixtures

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## Transport Analogy (flux)

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<b><u>Species A Mass</u></b> <i>in a mixture with B</i>	$j_{A,z} = -\rho D_{AB} \frac{\partial \omega_A}{\partial z}$	Fick's Law

Mass of species A diffusing in the z-direction, per area per time

- ✓ **Mass of species A** goes down a gradient in concentration of A *in a mixture*

Transport Analogy Reference:  
R. B. Bird, W. E. Stewart, E. N. Lightfoot,  
*Transport Phenomena*, 2<sup>nd</sup> edition, Wiley, 2002.

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Introduction to Diffusion and Mass Transfer in Mixtures

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There is a transport analogy but

- topics important to diffusion but not to fluid flow tend to be omitted or deemphasized (e.g. simultaneous diffusion and chemical reaction)
- Numerous topics unrelated to the transport law are deemphasized (in fluid mechanics non-Newtonian flow and heat transfer some aspects of macroscopic modeling)

*Transport Analogy Reference:*  
R. B. Bird, W. E. Stewart, E. N. Lightfoot,  
*Transport Phenomena*, 2<sup>nd</sup> edition, Wiley, 2002.

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Introduction to Diffusion and Mass Transfer in Mixtures

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## Transport Analogy (flux)

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- Numerous topics unrelated to the transport law are deemphasized (in fluid mechanics non-Newtonian flow and heat transfer some aspects of macroscopic modeling)

**How do we model diffusion?**



*Transport Analogy Reference:*  
R. B. Bird, W. E. Stewart, E. N. Lightfoot,  
*Transport Phenomena*, 2<sup>nd</sup> edition, Wiley, 2002.

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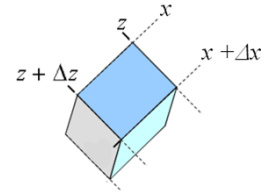
Introduction to Diffusion and Mass Transfer in Mixtures

**Modeling Diffusion/Mass Transfer:**

**Mass is Conserved**

- Both:
- overall mass
  - individual species' masses *in a mixture*

As was true in momentum transfer and heat transfer, solving problems with shell balances on individual control volumes is tricky, and it is easy to make errors.



Instead, we use the general equation, derived for all circumstances:

**Equation of Species A Mass Balance**  
(microscopic species mass balance)

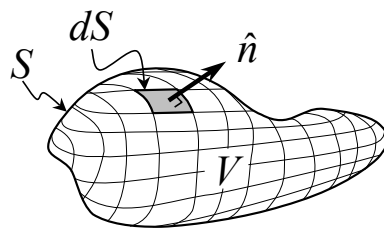
Recall the other microscopic balances, all written in terms of **Continuum Modeling**



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**Microscopic Momentum Balance:**

Equation of Motion



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

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

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

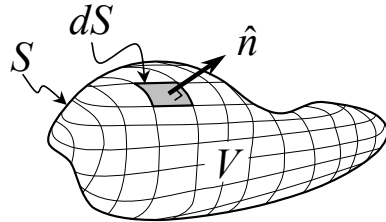
Navier-Stokes Equation;  
constant viscosity

Microscopic momentum balance is a vector equation.

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### Microscopic Energy Balance:

#### Equation of Thermal Energy



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

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

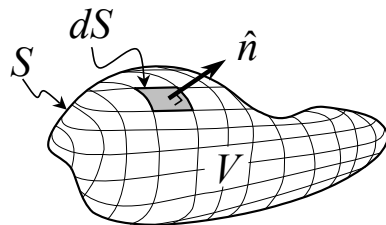
Gibbs notation: 
$$\rho \hat{C}_p \left( \frac{\partial T}{\partial t} + \underline{v} \cdot \nabla T \right) = k \nabla^2 T + S_e$$
 **Fourier conduction**

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

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### Microscopic Species A Mass Balance:

#### Equation of Species Mass Balance



Microscopic **species A mass** balance written on an arbitrarily shaped volume,  $V$ , enclosed by a surface,  $S$

Gibbs notation: 
$$\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v} \cdot \nabla \omega_A \right) = -\nabla \cdot \underline{j}_A + r_A$$
 **general mass transfer**

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

(written in terms of mass quantities; constant  $\rho D_{AB}$ )

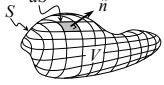
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### Introduction to Diffusion and Mass Transfer in Mixtures

**Recall Microscopic Momentum Balance:**

Equation of Motion



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

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

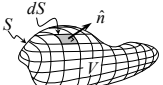
Gibbs notation:  $\rho \left( \frac{\partial \underline{v}}{\partial t} + \underline{v} \cdot \nabla \underline{v} \right) = -\nabla p + \mu \nabla^2 \underline{v} + \rho \underline{g}$  **Newtonian fluid**

Navier-Stokes Equation

Microscopic momentum balance is a vector equation.

**Microscopic Species A Mass Balance:**

Equation of Species Mass Balance



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

Gibbs notation:  $\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v} \cdot \nabla \omega_A \right) = -\nabla \cdot \underline{j}_A + r_A$  **general mass transfer**

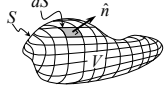
Gibbs notation:  $\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v} \cdot \nabla \omega_A \right) = \rho D_{AB} \nabla^2 \omega_A + r_A$  **Fickian diffusion**

(written in terms of mass quantities; constant  $\rho D_{AB}$ )

**Microscopic Balances:**

- All three have a convective term on the left-hand side (due to use of **control volume** and mass or per mass basis)
- All three have **two forms**, one including the flux and one with the transport law embedded

**Equation of Thermal Energy**



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

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

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

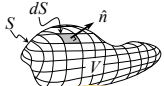
(incompressible fluid, constant pressure, neglect  $E_e, E_p$ , viscous dissipation)

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### Introduction to Diffusion and Mass Transfer in Mixtures

**Recall Microscopic Momentum Balance:**

Equation of Motion



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

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

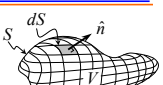
Gibbs notation:  $\rho \left( \frac{\partial \underline{v}}{\partial t} + \underline{v} \cdot \nabla \underline{v} \right) = -\nabla p + \mu \nabla^2 \underline{v} + \rho \underline{g}$  **Newtonian fluid**

Navier-Stokes Equation

Microscopic momentum balance is a vector equation.

**Microscopic Species A Mass Balance:**

Equation of Species Mass Balance



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

Gibbs notation:  $\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v} \cdot \nabla \omega_A \right) = -\nabla \cdot \underline{j}_A + r_A$  **general mass transfer**


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

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

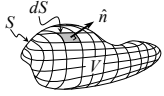
(incompressible fluid, constant pressure, neglect  $E_e, E_p$ , viscous dissipation)

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### Introduction to Diffusion and Mass Transfer in Mixtures

**Recall Microscopic Momentum Balance:**

**Equation of Motion**



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

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

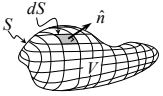
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Navier-Stokes Equation

Microscopic momentum balance is a vector equation.

**Microscopic Species A Mass Balance:**

**Equation of Species Mass Balance**



Microscopic **species A mass** balance written on an arbitrarily shaped volume,  $V$ , enclosed by a surface,  $S$ .

Gibbs notation:  $\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v} \cdot \nabla \omega_A \right) = -\nabla \cdot \underline{j}_A + r_A$  **general mass transfer**

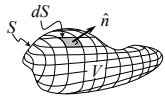
Gibbs notation:  $\rho \left( \frac{\partial \omega_A}{\partial t} + \underline{v} \cdot \nabla \omega_A \right) = \rho D_{AB} \nabla^2 \omega_A + r_A$  **Fickian diffusion**

(written in terms of mass quantities; constant  $\rho D_{AB}$ )

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**Equation of Thermal Energy**



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

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

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

(incompressible fluid, constant pressure, neglect  $E_e, E_p$ , viscous dissipation)

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### Introduction to Diffusion and Mass Transfer in Mixtures

## Microscopic species A mass balance

*in a mixture*

*Appears due to use of stationary coordinates (control volume)*

convection

rate of change

source

diffusion

(all directions)

Appears due to transport through a surface (control surface)

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

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

velocity must satisfy equation of motion, equation of continuity

The types of terms that appear are very much like similar mechanisms that we have seen in the other transport fields.

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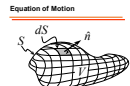
### Introduction to Diffusion and Mass Transfer in Mixtures

An underlying feature of these balances is the assumption that matter forms a **continuum**.

**momentum**

**Recall Microscopic Momentum Balance:**

**Equation of Motion**



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

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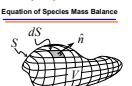
Navier-Stokes Equation

Microscopic momentum balance as a vector equation.

**species mass**

**Microscopic Species A Mass Balance:**

**Equation of Species A Mass Balance**



Microscopic **species A mass** balance written on an arbitrarily shaped volume,  $V$ , enclosed by a surface,  $S$ .

Gibbs notation:  $\rho \left( \frac{\partial \omega_A}{\partial t} + \mathbf{u} \cdot \nabla \omega_A \right) = -\nabla \cdot \mathbf{j}_A + \mathcal{R}_A$  **general mass transfer**

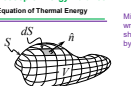
Gibbs notation:  $\rho \left( \frac{\partial \omega_A}{\partial t} + \mathbf{u} \cdot \nabla \omega_A \right) = \rho D_{AB} \nabla^2 \omega_A + \mathcal{R}_A$  **Fickian diffusion**

(written in terms of mass quantities, constant  $\rho D_{AB}$ )

**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:  $\rho \left( \frac{\partial E}{\partial t} + \mathbf{u} \cdot \nabla E \right) = -\nabla \cdot \mathbf{q} + S_v$  **general conduction**

Gibbs notation:  $\rho c_p \left( \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = k \nabla^2 T + S_p$  **Fourier conduction**

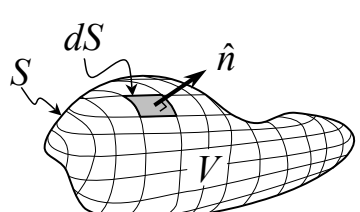
(incompressible fluid, constant pressure, neglect  $\dot{E}_v, \dot{E}_p$ , viscous dissipation)

To model diffusion and mass transfer within this familiar structure, we must adapt our notion of the **continuum**.

to accommodate aspects that are important in a mixture

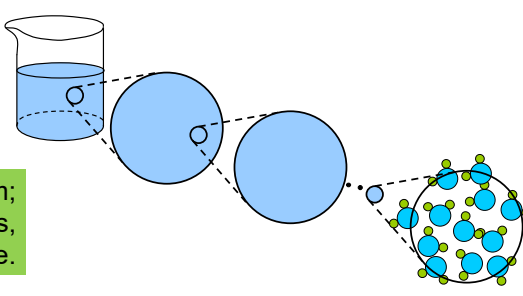
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### Continuum Modeling



*Microscopic* balances are written on an arbitrarily shaped microscopic volume,  $V$ , enclosed by a surface,  $S$

- A **continuum** is infinitely divisible
- Material properties ( $\mu, k, \rho$ ) are shared by all volume elements

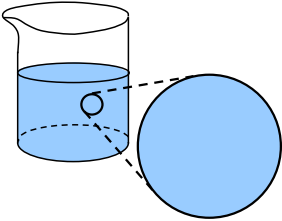


**BUT:** Real matter is *not* a continuum; at small enough length scales, molecules are discrete.


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Continuum Modeling

- A **continuum** is infinitely divisible
- Material properties ( $\mu, k, \rho$ ) are shared by all volume elements



- In a **binary mixture**, different pieces of matter have different material identities and different material properties

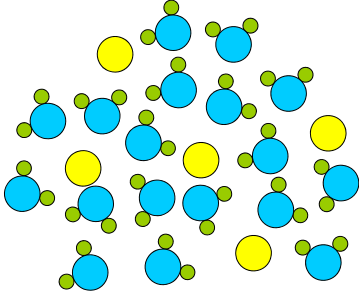
**Species A:** 

**Species B:** 

$x_A$ , mole fraction A

$x_B$ , mole fraction B

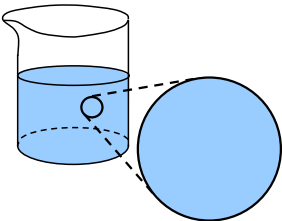
$C$ ,  $\frac{(\text{moles mixture})}{(\text{volume mixture})}$




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Continuum Modeling

- A **continuum** is infinitely divisible
- Material properties ( $\mu, k, \rho$ ) are shared by all volume elements



- In a **binary mixture**, different pieces of matter have different material identities and different material properties

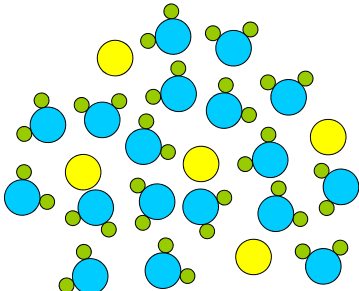
**Species A:** 

**Species B:** 

$\omega_A$ , mass fraction A

$\omega_B$ , mass fraction B

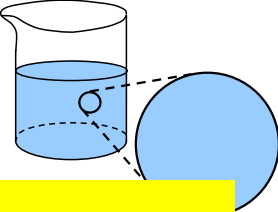
$\rho$ ,  $\frac{(\text{mass mixture})}{(\text{volume mixture})}$




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Continuum Modeling

- A **continuum** is infinitely divisible
- Material properties ( $\mu, k, \rho$ ) are shared by all volume elements



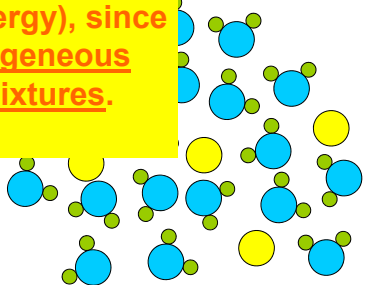
• In a **binary mixture**, matter have different chemical identities and different material properties

**Species A:**   $\omega_A$ , mass fraction A

**Species B:**   $\omega_B$ , mass fraction B

$$\rho, \frac{(\text{mass mixture})}{(\text{volume mixture})}$$

**We didn't have to deal with this before (momentum, energy), since we considered homogeneous materials and not mixtures.**



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Continuum Modeling


### Mass versus Moles


- A complication with the microscopic species mass balance is that we have been modeling systems as a **continuum**.
- In a continuum, material properties ( $\mu, k, \rho$ ) are shared by all volume elements.
- But now, we're interested in species A and B as separate entities.
- Chemical identity manifests as a distribution of atoms/molecules (or **moles** of either) and also as a distribution of **mass**.
- Molar and mass distributions **are not the same distribution**.

$$\omega_A, \text{ mass fraction } A$$

$$\omega_B, \text{ mass fraction } B$$

$$\rho, \frac{(\text{mass mixture})}{(\text{volume mixture})}$$

**Species A:** 

**Species B:** 

$$x_A, \text{ mole fraction } A$$

$$x_B, \text{ mole fraction } B$$

$$C, \frac{(\text{moles mixture})}{(\text{volume mixture})}$$

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Continuum Modeling

**Mass versus Moles**

$\omega_A$ , mass fraction A  
 $\omega_B$ , mass fraction B  
 $\rho$ ,  $\frac{(\text{mass mixture})}{(\text{volume mixture})}$

Species A:

Species B:

$x_A$ , mole fraction A  
 $x_B$ , mole fraction B  
 $C$ ,  $\frac{(\text{moles mixture})}{(\text{volume mixture})}$

**Should we express the diffusion of molecules in terms of moles or in terms of mass?**

**Does it matter?**

Answer? It depends.

**MASS!**

Fits well with previous microscopic balances (in a mixture,  $\underline{v}$  is the **mass average velocity**)

**MOLES!**

When reactions take place, reactions are naturally analyzed in terms of **moles**

This question has led to an increase of nomenclature.

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Species Fluxes

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

**Flux of what? And due to what mechanism?**

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

Microscopic species A mass balance

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

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

**Written relative to what velocity?**

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

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

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### 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)
- $\underline{m}_A$  – combined mass flux (includes convection and diffusion)
- $\underline{j}_A$  – mass flux (diffusion only)
- $\underline{J}_A$  – molar flux (diffusion only)

Microscopic species A mass balance

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

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

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- $\underline{J}_A$  – relative to the molar average velocity  $\underline{v}^*$

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

These different fluxes are a significant complication.

➔

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

➔

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### Microscopic species A mass balance—Five forms

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

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

➔

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

➔

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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
$n_A \equiv$ mass flux of species $A$ relative to stationary coordinates	$= \rho_A v_A = j_A + \rho_A v =$ <b>combined mass flux</b> relative to stationary coordinates $n_A + n_B = \rho v$
$J_A \equiv$ molar flux relative to a mixture's molar average velocity, $v^*$	$= c_A(v_A - v^*)$ $J_A + J_B = 0$
$N_A \equiv$ molar flux of species $A$ relative to stationary coordinates	$= c_A v_A = J_A + c_A v^* =$ <b>combined molar flux</b> 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	
$v \equiv \omega_A v_A + \omega_B v_B \equiv$ mass average velocity; same velocity as in the microscopic momentum and energy balances	
$v^* \equiv x_A v_A + x_B v_B \equiv$ molar average velocity	

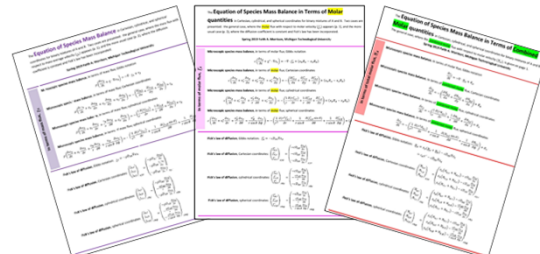
Part of the problem is that we have grown comfortable with the continuum, but now we are peering into the details of the continuum

➔

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

➔

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Various forms of Fick's Law (and the species mass balances that employ them)		
<p>Mass flux</p> $j_A = -\rho D_{AB} \nabla \omega_A$	<p>Molar flux</p> $J_A = -c D_{AB} \nabla x_A$	<p>Combined molar flux</p> $N_A = x_A(N_A + N_B) - c D_{AB} \nabla x_A$
		
<p>FRONT <a href="http://pages.mtu.edu/~fmorriso/cm3120/Homeworks_Readings.html">pages.mtu.edu/~fmorriso/cm3120/Homeworks_Readings.html</a></p>		

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

Let's jump in!

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

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

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## Diffusion and Mass Transfer QUICK START

Using the microscopic species mass balance in terms of combined molar flux and molar concentrations

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

QUICK START

$c_A [=] \frac{\text{moles } A}{\text{volume mix}} = x_A c =$  the concentration of  $A$  in the mixture

$\underline{N}_A [=] \frac{\text{moles } A}{\text{area} \cdot \text{time}} =$  combined molar flux of  $A$  (diffusion and convection) relative to stationary coordinates

$R_A [=] \frac{\text{moles } A}{\text{volume mix} \cdot \text{time}} =$  rate of production of  $A$  by reaction per unit volume mixture

$c [=] \frac{\text{moles mix}}{\text{volume mix}} =$  molar density of the mixture (for ideal gases  $c = \frac{n}{V} = \frac{P}{RT}$ )

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## Diffusion and Mass Transfer QUICK START

Using **Fick's law of diffusion** in terms of the same combined molar flux:

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

**QUICK START**

$\underline{N}_A [=] \frac{\text{moles } A}{\text{area} \cdot \text{time}}$  = combined molar flux of A (diffusion and convection) relative to stationary coordinates

$x_A [=] \frac{\text{moles } A}{\text{moles mix}}$  = mole fraction of A

$D_{AB} [=] \frac{\text{cm}^2}{\text{s}}$  = diffusion coefficient (diffusivity) of A in B

$c [=] \frac{\text{moles mix}}{\text{volume mix}}$  = molar density of the mixture (for ideal gases  $c = \frac{n}{V} = \frac{P}{RT}$ )

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## Diffusion and Mass Transfer QUICK START

Using **handy worksheets** to learn the common modeling assumptions

**QUICK START**

**The Equation of Species Mass Balance in Terms of Combined Molar Quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. The general case, where the **combined** flux with respect to molar velocity ( $\underline{N}_A$ ), is given on page 1. Spring 2019 Faith A. Morrison, Michigan Technological University

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

$$\frac{\partial N_A}{\partial t} = -\nabla \cdot (\underline{N}_A + N_A \underline{v})$$

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

$$\frac{\partial N_A}{\partial t} = -\left( \frac{\partial(N_A r)}{\partial r} + \frac{\partial(N_A z)}{\partial z} \right) + N_A \underline{v}$$

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

$$\frac{\partial N_A}{\partial t} = -\left( \frac{1}{r^2} \frac{\partial(r^2 N_A)}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(N_A \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial(N_A \phi)}{\partial \phi} \right) + N_A \underline{v}$$

**Fick's law of diffusion, Cartesian coordinates:**  $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

**Fick's law of diffusion, Cartesian coordinates:**  $\left( \frac{N_{A,r}}{N_{A,z}} \right) = \left( \frac{x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r}}{x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z}} \right)$

**Fick's law of diffusion, cylindrical coordinates:**  $\left( \frac{N_{A,r}}{N_{A,z}} \right) = \left( \frac{x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r}}{x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z}} \right)$

**Fick's law of diffusion, spherical coordinates:**  $\left( \frac{N_{A,r}}{N_{A,\theta}} \right) = \left( \frac{x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r}}{x_A(N_{A,\theta} + N_{B,\theta}) - cD_{AB} \frac{\partial x_A}{\partial \theta}} \right)$

**NOTES:**

- If component A has no sink,  $\dot{N}_A = 0$ .
- If A diffuses through stagnant B,  $\underline{N}_B = 0$ .
- If a binary mixture of A and B are undergoing steady equimolar counterdiffusion,  $\underline{N}_A = -\underline{N}_B$ .
- If, for example, two moles of A diffuse to a surface at which a rapid, irreversible reaction converts it to one mole of K, then at steady state  $-0.5\underline{N}_A = \underline{N}_K$ .

$c x_A = c_A = \frac{N_A}{V} = \frac{1}{V} \sum_i N_{A,i}$  (units:  $c [=] \frac{\text{mol}}{\text{m}^3}$ )

$\underline{J}_A$  = molar flux relative to a mixture's molar average velocity

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

$\underline{N}_A = c_A \underline{v}_A + c_A \underline{v}^*$  = **combined** flux relative to stationary coordinates

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

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

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

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

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Microscopic Species Mass Balance
QUICK START

**The Equation of Species Mass Balance in Terms of Combined Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. The general case, where the combined molar flux with respect to molar velocity ( $\underline{N}_A$ ), is given on page 1.  
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In terms of total molar flux,  $\underline{N}_A$

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

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

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

$$\frac{\partial c_A}{\partial t} = -\left(\frac{\partial N_{A,x}}{\partial x} + \frac{\partial N_{A,y}}{\partial y} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

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

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r} \frac{\partial(rN_{A,r})}{\partial r} + \frac{1}{r} \frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

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

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r^2} \frac{\partial(r^2 N_{A,r})}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(N_{A,\theta} \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial N_{A,\phi}}{\partial \phi}\right) + R_A$$

Note: this handout is on the web

[pages.mtu.edu/~fmorriso/cm3120/Homeworks\\_Readings.html](http://pages.mtu.edu/~fmorriso/cm3120/Homeworks_Readings.html)

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Fick's Law of Diffusion in terms of Combined Molar Flux  $\underline{N}_A$ 
QUICK START

**Fick's law of diffusion, Gibbs notation:**  $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

$$= c_A \underline{v}^* - cD_{AB}\nabla x_A$$

**Fick's law of diffusion, Cartesian coordinates:**

$$\begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB} \frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB} \frac{\partial x_A}{\partial y} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$$

**Fick's law of diffusion, cylindrical coordinates:**

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,z} \end{pmatrix}_{r\theta z} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$$

**Fick's law of diffusion, spherical coordinates:**

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r \sin \theta} \frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

Note: this handout is on the web

[pages.mtu.edu/~fmorriso/cm3120/Homeworks\\_Readings.html](http://pages.mtu.edu/~fmorriso/cm3120/Homeworks_Readings.html)

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QUICK START

Handy reminder of definitions and relationships among mixture quantities

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

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

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

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

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

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

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

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

Note: this  
handout is  
on the web

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

[pages.mtu.edu/~fmorriso/cm3120/Homeworks\\_Readings.html](http://pages.mtu.edu/~fmorriso/cm3120/Homeworks_Readings.html)
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QUICK START

**Example:** Water (40°C, 1.0 atm) slowly and steadily evaporates into nitrogen (40°C, 1.0 atm) from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. The geometry is as shown in the figure. **What is the rate of water evaporation?**

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**Interrogating the problem:**

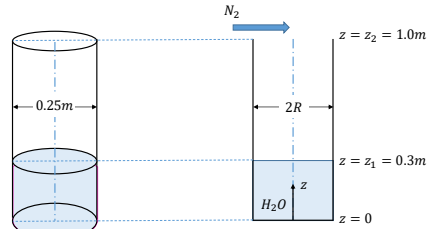
*Why does the water evaporate?*

*What limits the rate of evaporation?*

*What could be done to accelerate the evaporation?*

*What could be done to slow down the evaporation?*

**QUICK START**  
**Example:** Water ( $40^\circ\text{C}$ ,  $1.0\text{ atm}$ ) slowly and steadily evaporates into nitrogen ( $40^\circ\text{C}$ ,  $1.0\text{ atm}$ ) 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. **What is the rate of water evaporation?**

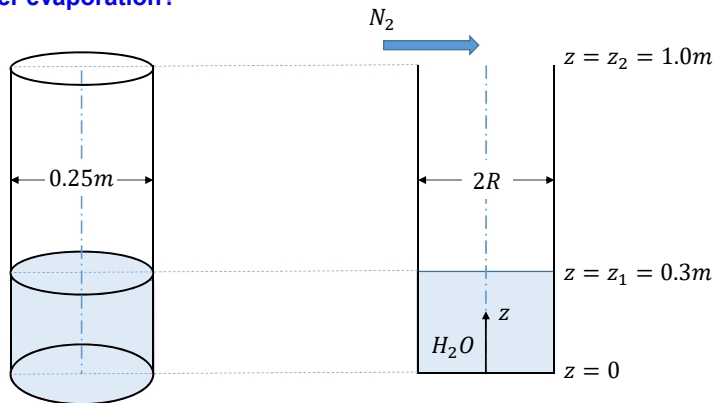


*What is the driving physics?*

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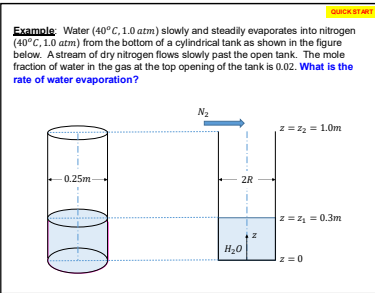
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**QUICK START**  
**Example:** Water ( $40^\circ\text{C}$ ,  $1.0\text{ atm}$ ) slowly and steadily evaporates into nitrogen ( $40^\circ\text{C}$ ,  $1.0\text{ atm}$ ) from the bottom of a cylindrical tank as shown in the figure below. A stream of 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?**



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Solve.

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