CM3120: Module 3

Diffusion and Mass Transfer I

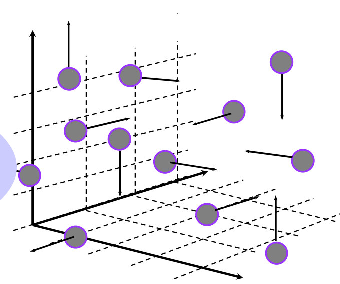
I. Introduction to diffusion/mass transfer
II. Classic diffusion and mass transfer—Quick Start a): 1D Evaporation
III. Classic diffusion and mass transfer—Quick Start b): 1D Radial droplet
IV. Cycle back: Fick's mass transport law
V. Microscopic species A mass balance
VI. Classic diffusion and mass transfer—c): 1D Mass transfer with chemical reaction

 1

CM3120: Module 3

Module 3 Lecture I

Introduction to Diffusion and Mass Transfer



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

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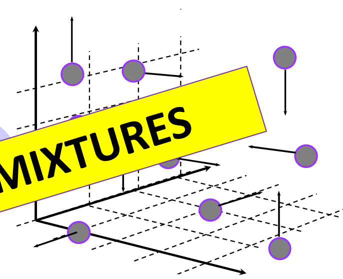
CM3120: Module 3

Module 3 Lecture I

Introduction to Diffusion and Mass Transfer in MIXTURES



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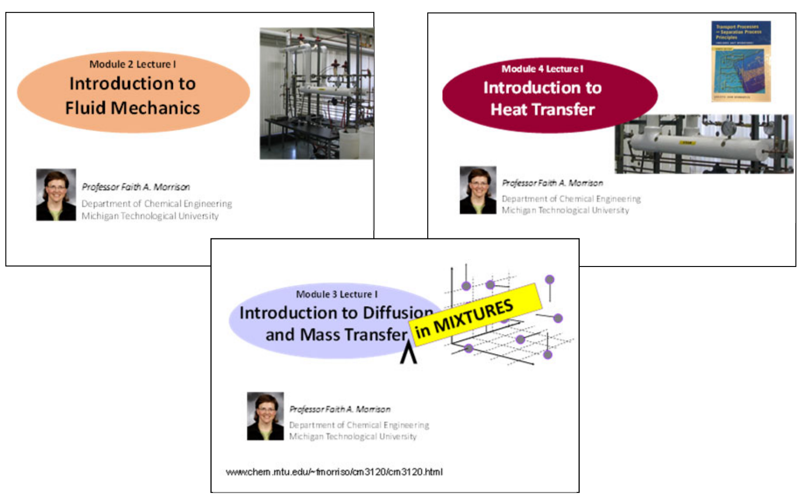
 3

We take a moment to reflect on **Transport** and its relationship to **Unit Operations** and the field of **Chemical Engineering**.



Transport: What have we learned? (and why were these topics chosen?). The answers will guide the choice of topics that we discuss in this third part, species A mass transfer.

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Ref: https://www.sciencehistory.org/historical-profile/arthur-d-little-william-h-walker-and-warren-k-lewis

Unit Operations

The term “unit operation” was coined by the founders of chemical engineering in the late 1800s.

Chemical processes may be broken down into basic steps that bring about physical or chemical change. These steps are called “unit operations.”

Chemical engineering unit operations may be divided into six classes:

1. **Fluid flow processes** including fluids transportation, filtration, mixing, and solids fluidization.
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3. **Mass transfer processes** including gas absorption, distillation, extraction, adsorption, membrane separation, crystallization & drying
4. **Thermodynamic processes** including refrigeration, water cooling, and gas liquefaction.
5. **Reaction** including homogeneous and catalytic reactors
6. **Mechanical processes** including solids transportation, crushing & pulverization, and screening & sieving.

Ref: Wikipedia, Unit Operations

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Unit Operations

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Ref: Wikipedia, Unit Operations

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The six classes of unit operations line up with classes in the ChemE Curriculum

Within each course taught, we cover the science, knowledge, and skills that allow us to address specific *engineering purposes*

(engineering purposes = quantities needed to design and operate the unit)

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Engineering purposes

1. Fluids: $\Delta p(Q), \mathcal{F}, \mathcal{T}, W_{s,on}$
2. Heat: $\dot{Q}, \mathcal{R}, U, NTU, \mathcal{A}_{xfer}$
3. Mass: $N_A, \underline{J}_A, \mathrm{H}_{\text{column}}, \mathrm{D}, \mathrm{N}_{\text{stages}}$
4. Thermo: phase relations, PVT, $\mathcal{Q}_H, \mathcal{Q}_C, \mathcal{W}_{on}$
5. Reaction: $f_{rxn}, V_{rxr}, \xi, r_A, RTD$

Pulling together the physics (how the world works) for these units is the subject of the field of chemical engineering

The six classes of unit operations line up with classes in the ChemE Curriculum

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Engineering purposes

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4. Thermo: phase relations, PVT, $\mathcal{Q}_H, \mathcal{Q}_C, \mathcal{W}$
5. Reaction: f, V, ξ, r_A, RTD

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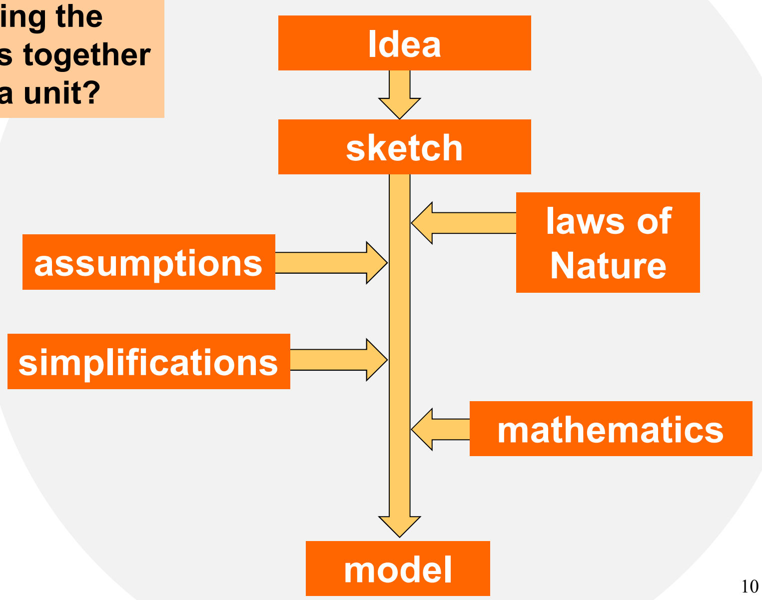
What is the *process* for pulling the physics together for a unit?



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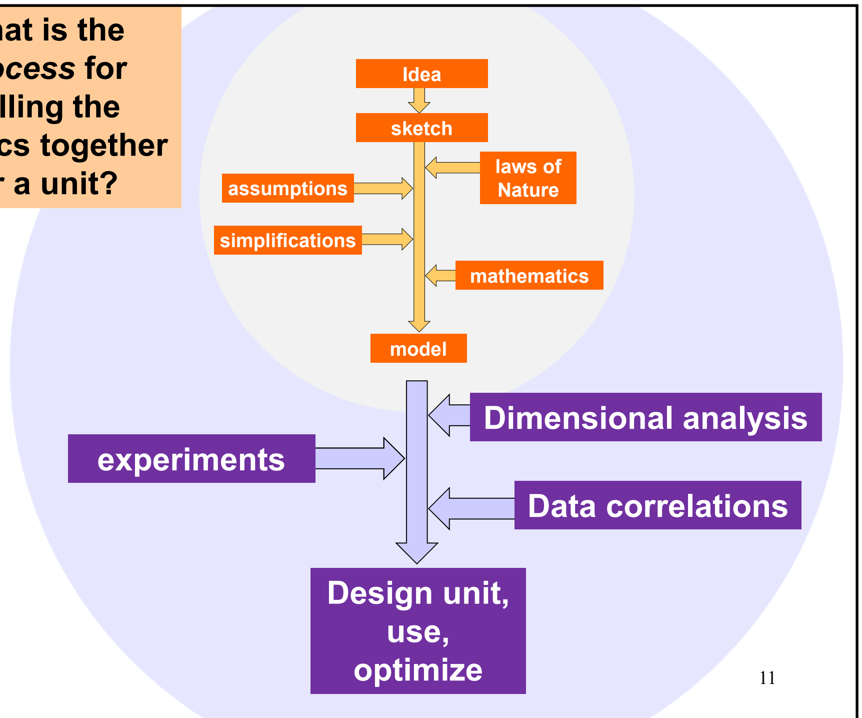
What is the *process* for pulling the physics together for a unit?



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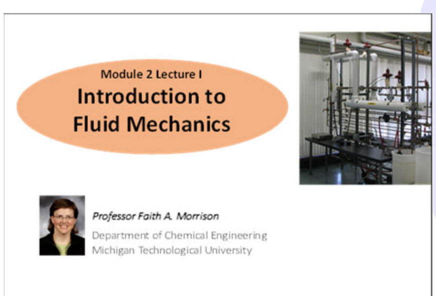
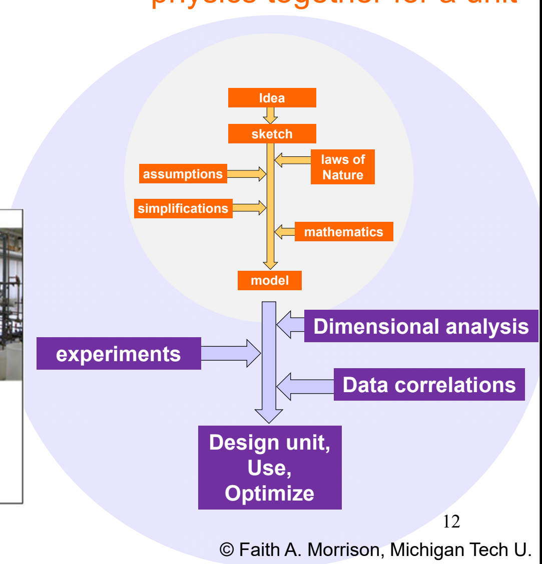
Let’s get specific

How did this process work for units dominated by fluid mechanics?



Process for pulling the physics together for a unit



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Fluid Flow Processes

Engineering Purposes:

- **Pipe flow, laminar/turbulent**
- **Device friction losses**
- **Centrifugal pumping curves**
- **Shaft work $W_{s,on}$**
- **Device $\Delta p(Q)$**
- **Mixing/settling**
- **Fluidized bed**
- **Filtration/packed beds**

Image from www.directindustry.com

Image from: www.processindustryforum.com

Image from: www.directindustry.com

Knowledge and Skills

1. Continuum
2. Mass, energy, momentum balances
3. Momentum flux ∝ velocity gradient
4. Transfers at boundaries, $\mathcal{F}_{drag}$
5. Dimensional analysis and data correlations, f, C_D
6. Classics: Internal/external flows, boundary layers

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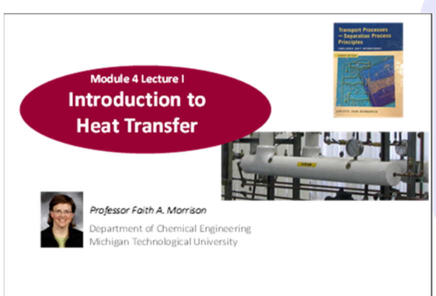
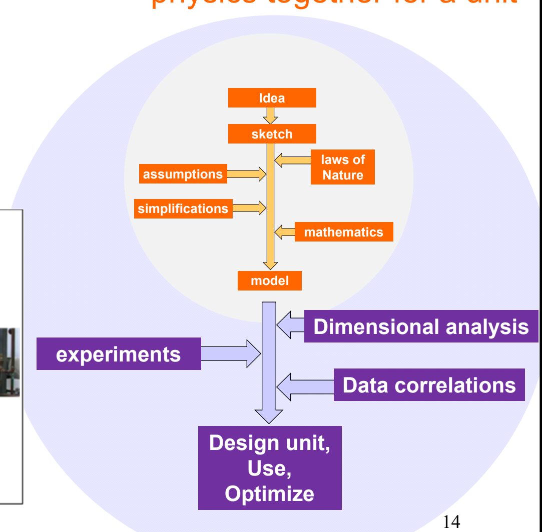
Next:

How did this process work for units dominated by heat transfer?



Process for pulling the physics together for a unit



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Heat Transfer Processes

Engineering Purposes:

- **Heat exchangers**
- **Evaporators**
- **Oven/Furnace design**
- **Radiators for cooling**
- **Condensers**
- **Dryers**

Knowledge and Skills

1. Continuum
2. Mass, energy balances, fluid flow fundamentals
3. Heat flux $\propto$ temperature gradient
4. Transfers at boundaries, h
5. Dimensional analysis and data correlations Nu, Bi
6. Thermo: Single condensable component
7. Classics: Internal/external resistance, forced, natural, radiation, boundary layers

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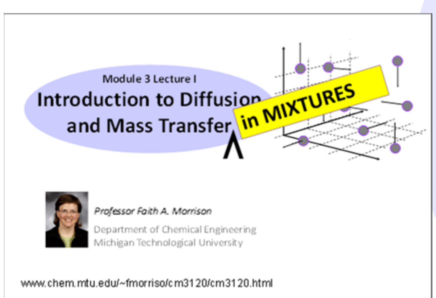
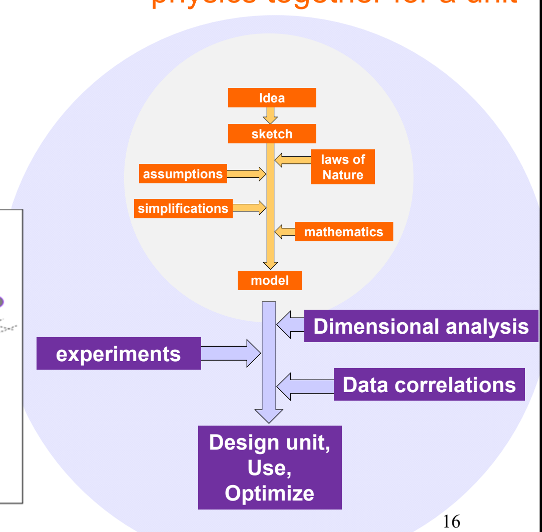
And now:

How does this process work for units dominated by mass transfer?



Process for pulling the physics together for a unit



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Species A Mass Transfer Processes

Engineering Purposes:

- **Distillation**
- **Gas absorption**
- **Extraction**
- **Membrane separation**

Knowledge and Skills

1. Continuum, mixtures
2. Mass, species A mass, energy balances, fluid flow fundamentals
3. Species A flux ∝ concentration gradient
4. Transfers at boundaries, k_x
5. Dimensional analysis and data correlations $\mathrm{Nu}_{AB}, \mathrm{Sh}$
6. Thermo: Binary phase equilibria
7. Classics: Stagnant layers, constant molar overflow, equimolar counter diffusion, film model, penetration model, boundary layers

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Species A Mass Transfer Processes

Engineering Purposes:

- **Distillation**
- **Gas absorption**
- **Extraction**
- **Membrane separation**

Modules 3, 4 will cover these topics for species A mass transfer

Knowledge and Skills

1. Continuum, mixtures
2. Mass, species A mass, energy balances, fluid flow fundamentals
3. Species A flux ∝ concentration gradient
4. Transfers at boundaries, k_x
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CM3120: Module 3

Diffusion and Mass Transfer I

I. Introduction to diffusion/mass transfer
II. Classic Diffusion and Mass Transfer—Quick Start
  a. Quick Start 1: 1D Evaporation
  b. Quick Start 2: 1D Radial droplet, surface reaction
III. Cycle back: Fick's mass transport law
IV. Microscopic species A mass balance
V. Classic Diffusion and Mass Transfer
  c. 1D mass transfer with chemical reaction

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CM3120: Module 3

Module 3 Lecture I

Introduction to Diffusion and Mass Transfer

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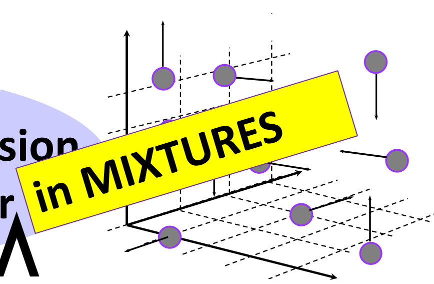

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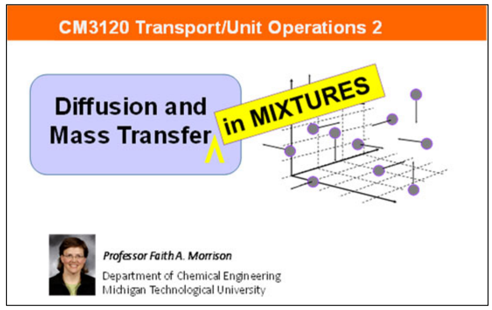
Introduction to Diffusion and Mass Transfer in Mixtures

For the first time we are concerned with *mixtures* and specifically with components of a mixture treated as separate entities



For flow and heating/cooling we just needed to know how to *average* material properties $(\mu, k, \hat{C}_p, \text{etc.})$ to deal with a mixture

When ***mass transfer*** is taking place, individual species are moving separately

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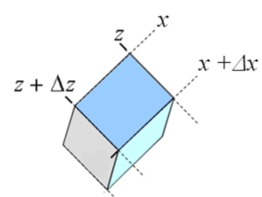
Introduction to Diffusion and Mass Transfer in Mixtures

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, microscopic balance 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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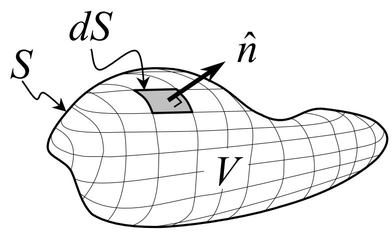
Microscopic Momentum Balance:

Equation of Motion



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

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

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

Navier-Stokes Equation; constant density, viscosity

Microscopic momentum balance is a vector equation.

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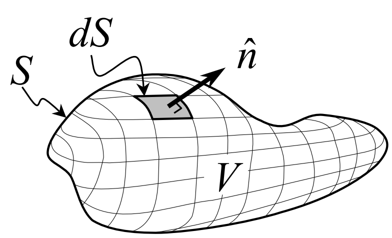
Microscopic Energy Balance:

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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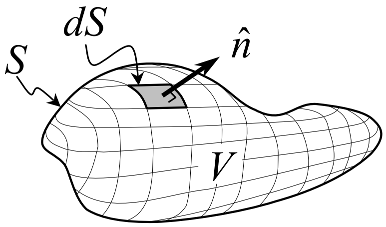
Microscopic Species A Mass Balance:

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

(written in terms of mass quantities; constant ρD_{AB})

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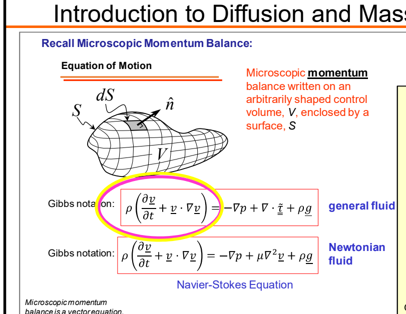
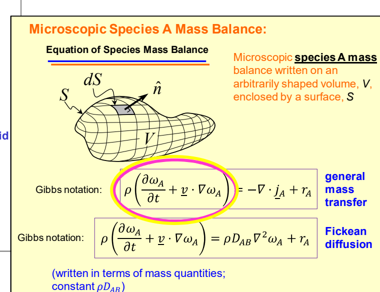
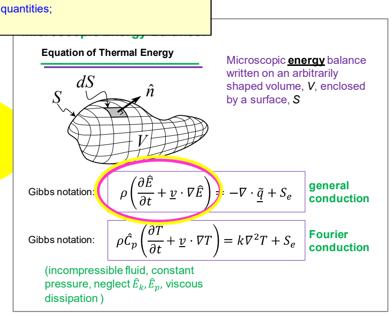
Introduction to Diffusion and Mass Transfer in Mixtures







Microscopic Balances:

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

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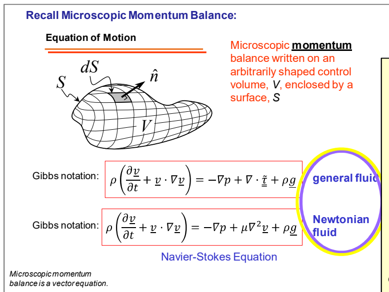
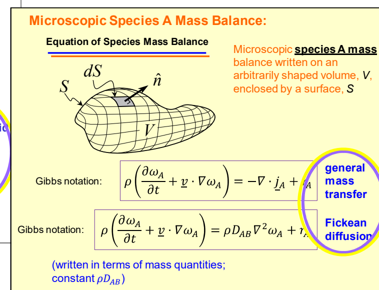
Introduction to Diffusion and Mass Transfer in Mixtures





Microscopic Balances:

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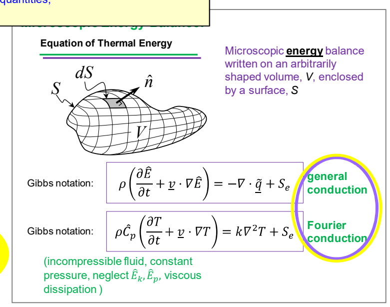
- **All three have <u>two forms</u>, one including the flux and one with the transport law embedded**



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Introduction to Diffusion and Mass Transfer in Mixtures

Transport Laws (flux proportional to driving gradient, "ordinary" transport)

<u>Momentum</u>

$$-\tilde{\tau}_{yz}=-\mu\frac{\partial v_y}{\partial z}$$ Newton's Law of Viscosity

<u>Heat</u>

$$\frac{q_z}{A}=-k\frac{\partial T}{\partial z}$$ Fourier's Law of Conduction

<u>Species A Mass</u>

in a mixture with B $$j_{A,z}=-\rho D_{AB}\frac{\partial \omega_A}{\partial z}$$ Fick's Law of Diffusion

- ✓ **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*

These "ordinary" transport processes are due to Brownian motion

R. B. Bird, W. E. Stewart, E. N. Lightfoot, *Transport Phenomena*, 2nd ed,, 2002. p. xxi

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Introduction to Diffusion and Mass Transfer in Mixtures

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Unit Operations

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5. **Reaction** including homogeneous and catalytic reactors
6. **Mechanical processes** including solids transportation, crushing & pulverization, and screening & sieving.

Examples of units involving “non-ordinary” transport processes:

- Water cooling (Thermodynamics)
- Refrigeration (Thermodynamics)
- Gas liquefaction (Thermodynamics)
- Extrusion, coating, food processing (Non-newtonian fluid mechanics)
- Solids processing (minerals processing)
- Protein centrifugation (forced diffusion)
- Ultracentrifugation (pressure diffusion)
- Isotopic separation (thermal diffusion)
- Electrodialysis (electropotential gradient)

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Introduction to Diffusion and Mass Transfer in Mixtures

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- Protein centrifugation (forced diffusion)
- Ultracentrifugation (pressure diffusion)
- Isotopic separation (thermal diffusion)
- Electrodialysis (electropotential gradient)

Note:
- There are many;
- They are important

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Introduction to Diffusion and Mass Transfer in Mixtures

Transport Laws (flux proportional to driving gradient, "ordinary" transport)

Momentum

$$-\tilde{\tau}_{yz} = -\mu \frac{\partial v_y}{\partial z}$$ Newton's Law of Viscosity

Heat

$$\frac{q_z}{A} = -k \frac{\partial T}{\partial z}$$ Fourier's Law of Conduction

Species A Mass

in a mixture with B

$$j_{A,z} = -\rho D_{AB} \frac{\partial \omega_A}{\partial z}$$ Fick's Law of Diffusion

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*

What is ordinary diffusion and how do we model it?

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Introduction to Diffusion and Mass Transfer in Mixtures

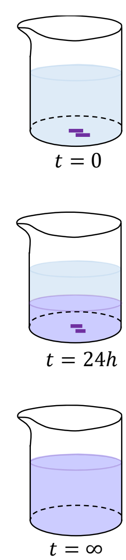
Diffusion

- Is the mixing process caused by random molecular motion (Brownian motion).
- Is ***slow***
- Since it is slow, it acts over short distances

Diffusion progresses at a rate of
- $\sim 5 cm/min$ (gases)
- $\sim 0.05 cm/min$ (liquids)
- $\sim 10^{-5} cm/min$ (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



Diffusion is slow

References:
- E. L. Cussler, *Diffusion: Mass Transfer in Fluid Systems*, 3rd ed, Cambridge University Press, 2016.
- R. B. Bird, W. E. Stewart, E. N. Lightfoot, *Transport Phenomena*, 2nd ed, 2002.
- C. J. Geankoplis, *Transport Processes and Separation Process Principles*, 4th Edition, Prentice Hall, 2003 p. xxi

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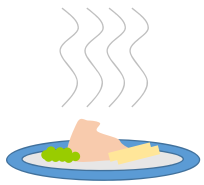
Introduction to Diffusion and Mass Transfer in Mixtures

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



Diffusion progresses at a rate of
- $\sim 5 cm/min$ (gases)
- $\sim 0.05 cm/min$ (liquids)
- $\sim 10^{-5} cm/min$ (solids)

Was it diffusion?

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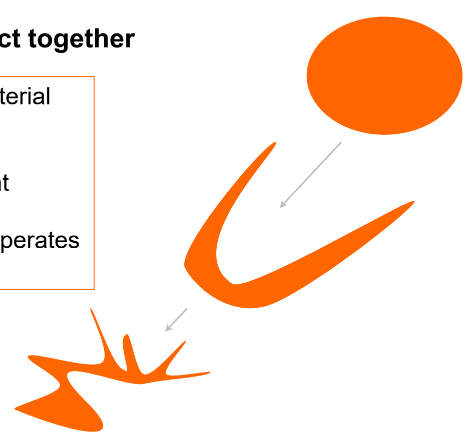
Introduction to Diffusion and Mass Transfer in Mixtures

Mass Transfer

Convection and Diffusion act together

- 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



Cussler p. 1

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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

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

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

rate of change

diffusion (all directions)

Appears due to diffusive transport through a surface (control surface)

Mass-average velocity must satisfy equation of motion, equation of continuity

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Introduction to Diffusion and Mass Transfer in Mixtures

Microscopic species A mass balance *in a mixture*

convection

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

diffusion (all directions)

In species A mass transfer, it can be hard to separate convection and diffusion

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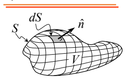
Introduction to Diffusion and Mass Transfer in Mixtures

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

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

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

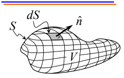
Navier-Stokes Equation

Microscopic momentum balance is a vector equation.

species mass

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

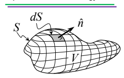
Gibbs notation: $\rho\left(\frac{\partial \omega_A}{\partial t}+\underline{v}\cdot\nabla\omega_A\right)=\rho D_{AB}\nabla^2\omega_A+r_A$ Fickean diffusion

(written in terms of mass quantities; constant ρD_{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: $\rho\left(\frac{\partial \hat{E}}{\partial t}+\underline{v}\cdot\nabla\hat{E}\right)=-\nabla\cdot\underline{\tilde{q}}+S_e$ general conduction

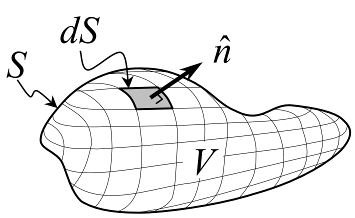
Gibbs notation: $\rho\hat{C}_p\left(\frac{\partial T}{\partial t}+\underline{v}\cdot\nabla T\right)=k\nabla^2 T+S_e$ Fourier conduction

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

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

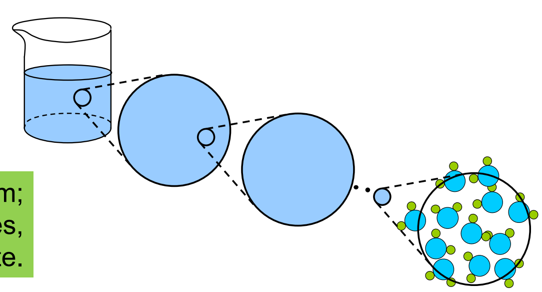
to accommodate circumstances that are important in a mixture undergoing internal mass transport

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 (μ, k, ρ) are shared by all volume elements

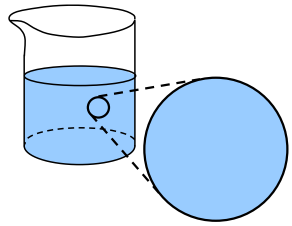


BUT:

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

Continuum Modeling

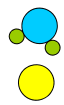
- A **continuum** is infinitely divisible
- Material properties (μ, k, ρ) are shared by all volume elements



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

Species A:

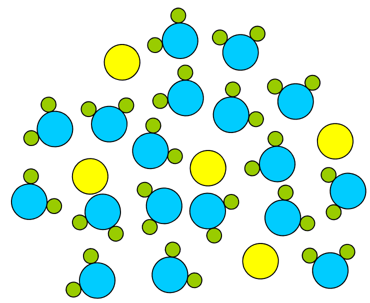
Species B:



x_A, mole fraction A

x_B, mole fraction B

$c, \ \dfrac{\text{(moles mixture)}}{\text{(volume mixture)}}$



MOLAR basis

Moles are easier when reactions occur…

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Continuum Modeling

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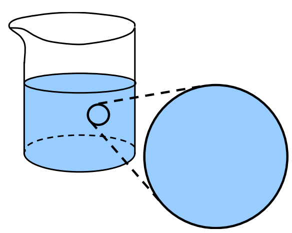

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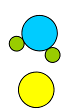
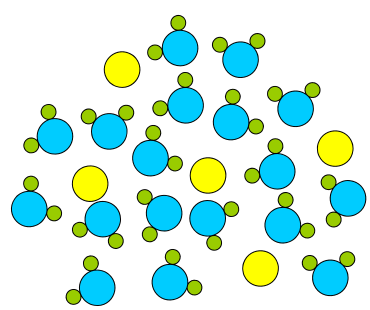


ω_A, mass fraction A

ω_B, mass fraction B

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



MASS basis

Only **mass** is conserved…

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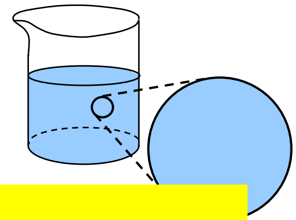
Continuum Modeling

- A **continuum** is infinitely divisible
- Material properties (μ, k, ρ) are shared by all volume elements



- In a **binary m** matter have di and different m

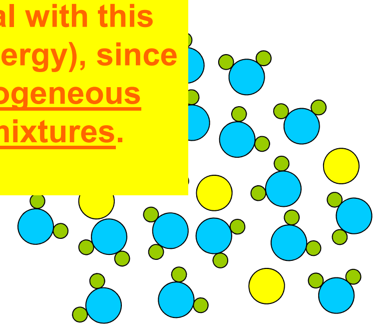
Species A:

Species B:

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

ω_B, mass fraction B

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



MASS basis

Only **mass** is conserved…

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Continuum Modeling

Mass versus Moles

- A complication with the microscopic species mass balance is that we are accustomed to modeling systems as a **continuum**.
- In a continuum, material properties (μ, k, ρ) 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.**

x_A, mole fraction A

x_B, mole fraction B

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

Species A:

Species B:

ω_A, mass fraction A

ω_B, mass fraction B

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

MOLAR basis

Moles are easier when reactions occur…

Only **mass** is conserved…

MASS basis

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Continuum Modeling

Mass versus Moles

ω_A, mass fraction A

ω_B, mass fraction B

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

Species A:

Species B:

x_A, mole fraction A

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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?

Answers? a) It depends. b) Yes.

MASS! Fits well with previous microscopic balances (in a mixture, $\underline{v}$ is the **mass average velocity**); easier to "slash and burn"

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

This tradeoff has led to an unavoidable confusion 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 both convection and diffusion)

$\underline{n}_A$ – combined mass flux (includes both convection and diffusion)

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

$\underline{J}_A^*$ – molar flux (diffusion only)

Microscopic species A mass balance

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

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

Written relative to what velocity?

$\underline{N}_A$ – relative to stationary coordinates

$\underline{n}_A$ – relative to stationary coordinates

$\underline{j}_A$ – relative to the mass average velocity $\underline{v}$

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

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

BSL2, p552

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Species Fluxes

It can be hard to separate convection and diffusion

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BSL2, p552

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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: $c x_A = c_A = \frac{1}{M_A}(\rho_A) = \frac{1}{M_A}(\rho \omega_A)$

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

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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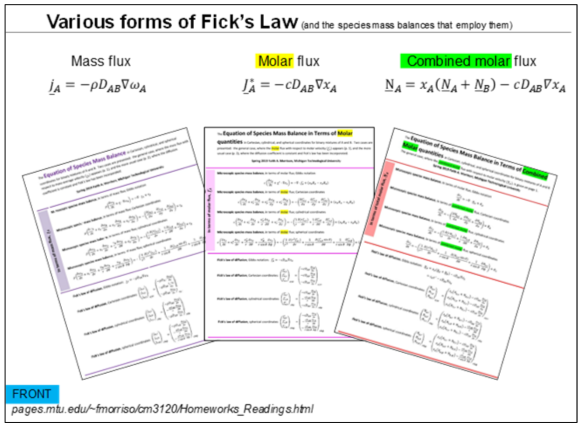

We will be introduced to handy worksheets and to the common assumptions and boundary conditions (just like in momentum and energy balances)

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

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

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

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.

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

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

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

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

$c [=] \frac{moles\ mix}{volume\ mix} =$ 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

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

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

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

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

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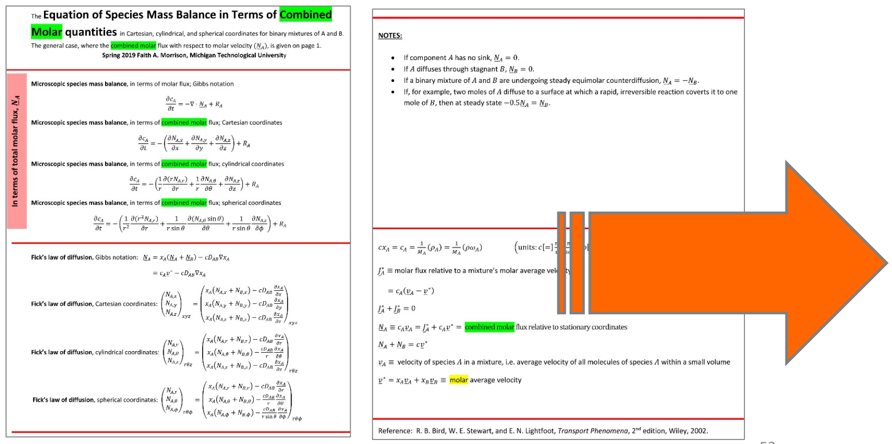
Diffusion and Mass Transfer QUICK START

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

QUICK START



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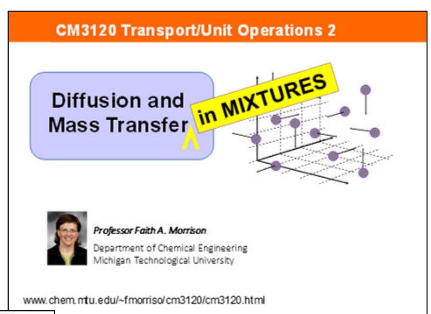
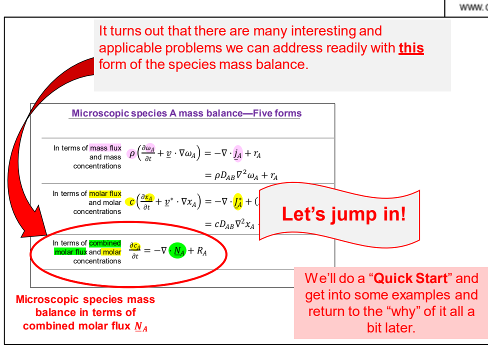
https://pages.mtu.edu/~fmorriso/cm3120/species_mass_bal_3_combinedmolarflux.pdf

Diffusion and Mass Transfer





QUICK START

(to problem solving)

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