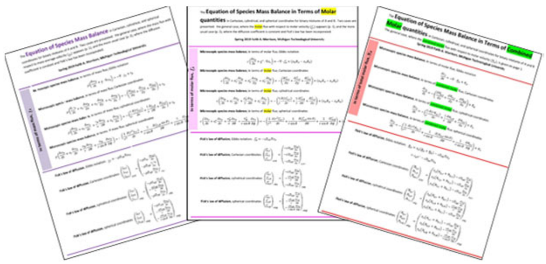
Let's put this to use



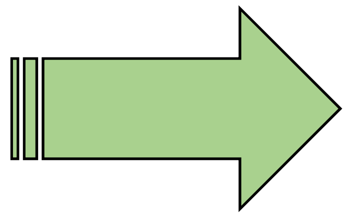
Various forms of the Microscopic Species A Mass Balance

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



1

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

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

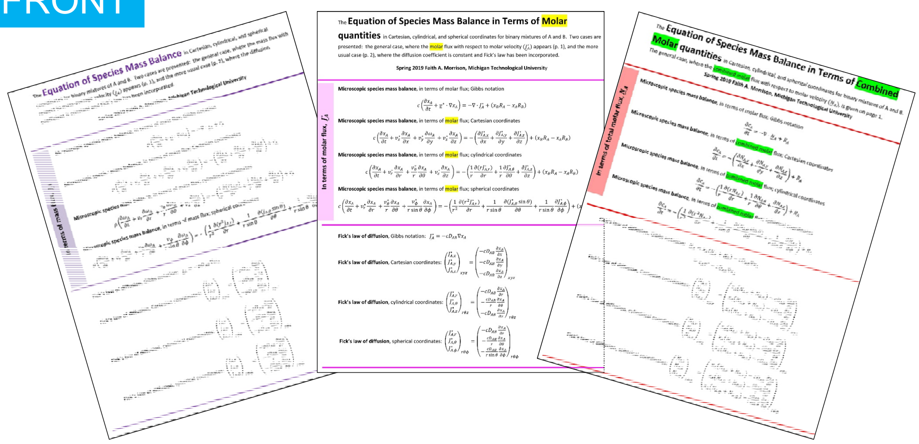
(The $\underline{N}_A$ version, with Fick's law substituted in, provides little advantage.)

2

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

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

FRONT



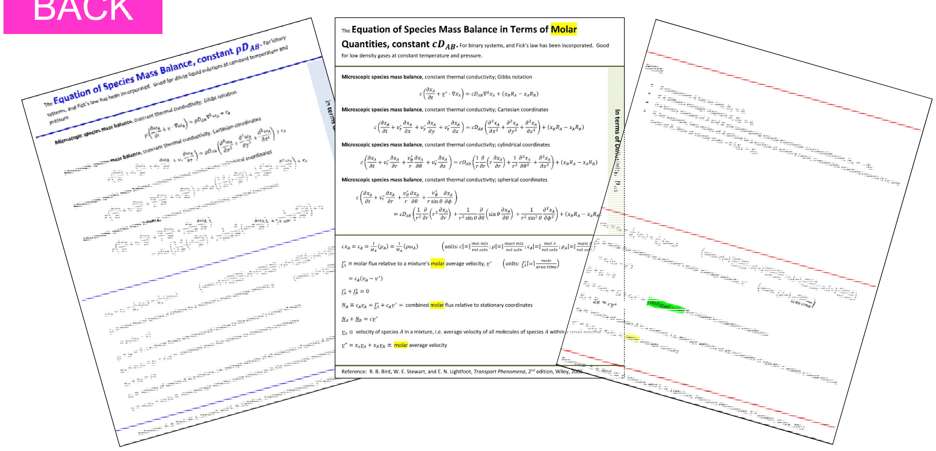
pages.mtu.edu/~fmorriso/cm3120/Homeworks_Readings.html

3

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

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

BACK



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

4

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

5

1D Steady Diffusion—Heterogeneous Chemical Reaction

Example: Heterogeneous catalysis in a reactor

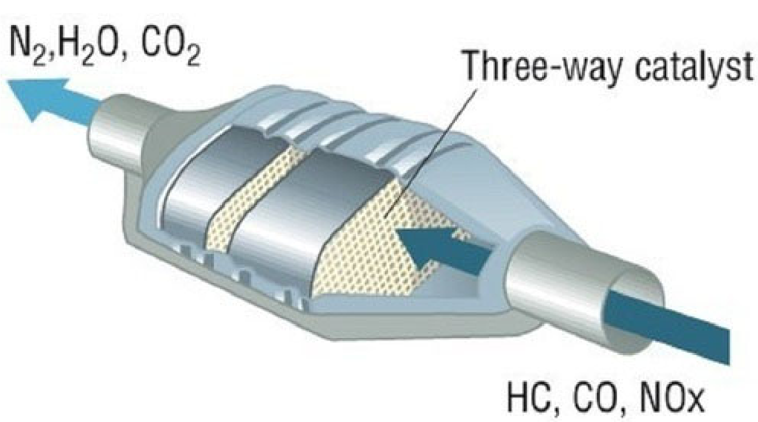


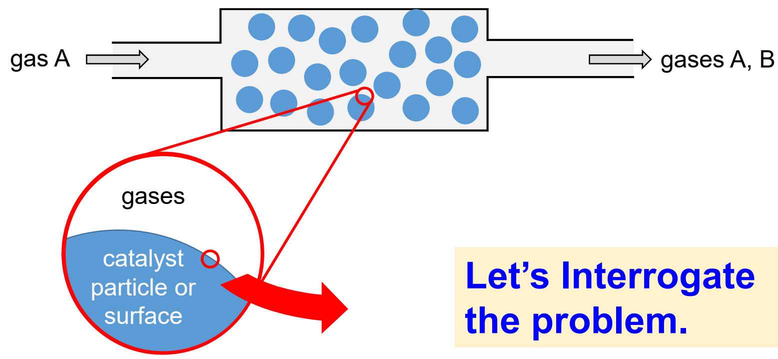
Image source: https://www.indiamart.com/proddetail/three-way-catalytic-converter-16802815188.html

BSL2, p552

6

1D Steady Diffusion—Heterogeneous Chemical Reaction

Example: Heterogeneous catalysis



Let's Interrogate the problem.

An irreversible, instantaneous chemical reaction $(2A \rightarrow B)$ takes place at a catalyst surface in a reactor as shown. How might mass transfer affect the observed rate of reaction?

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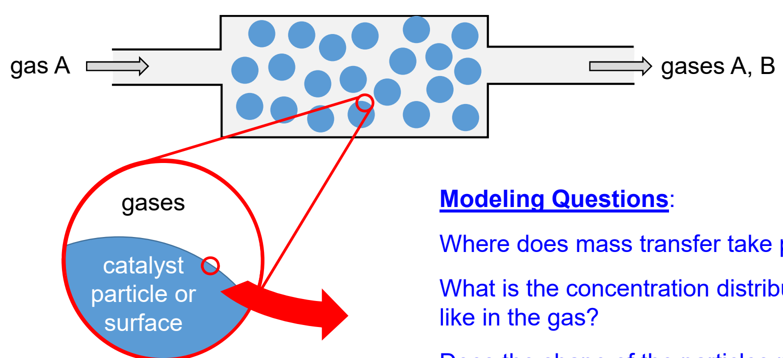
1D Steady Diffusion—Heterogeneous Chemical Reaction

Example: Heterogeneous catalysis



Modeling Questions:

Where does mass transfer take place?

What is the concentration distribution like in the gas?

Does the shape of the particles matter?

What is the impact of the overall (bulk) flow?

What should be our first modeling problem?

An irreversible, instantaneous chemical reaction $(2A \rightarrow B)$ takes place at a catalyst surface in a reactor as shown. How might mass transfer affect the observed rate of reaction?

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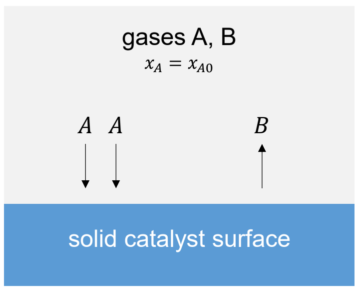
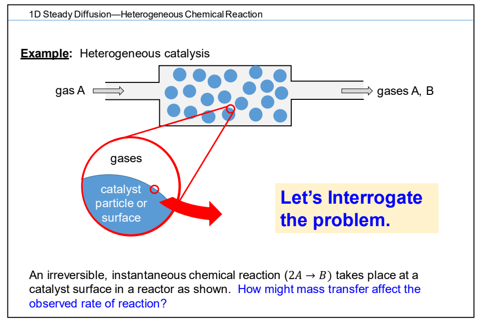
 8

1D Steady Diffusion—Heterogeneous Chemical Reaction

Example: Heterogeneous catalysis

An irreversible, instantaneous chemical reaction ($2A \rightarrow B$)





More Modeling Questions:

How fast will this happen?

Does it depend on the reaction rate?

What else does it depend on?

What can we learn about the unit's mass transfer character?

BSL2, p552

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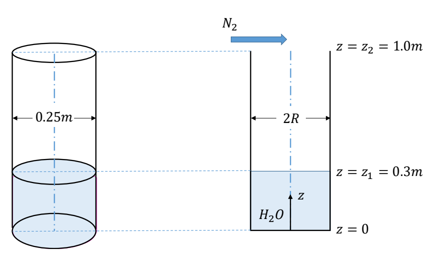
1D Steady Diffusion—Heterogeneous Chemical Reaction

Modeling Inspiration:

There may be a stagnant region between the *source* and *sink* that must be traversed.

QUICK START

Example: Water ($40^oC, 1.0\ atm$) slowly and steadily evaporates into nitrogen ($40^oC, 1.0\ atm$) 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. **What is the rate of water evaporation?**



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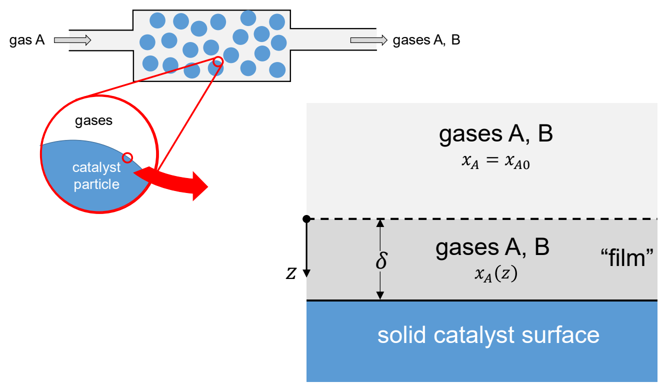
1D Steady Diffusion—Heterogeneous Chemical Reaction

Example: Heterogeneous catalysis

Use a "*film model*"



A stagnant region that must be traversed.

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

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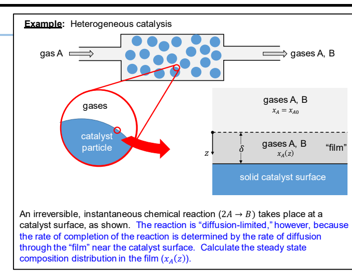
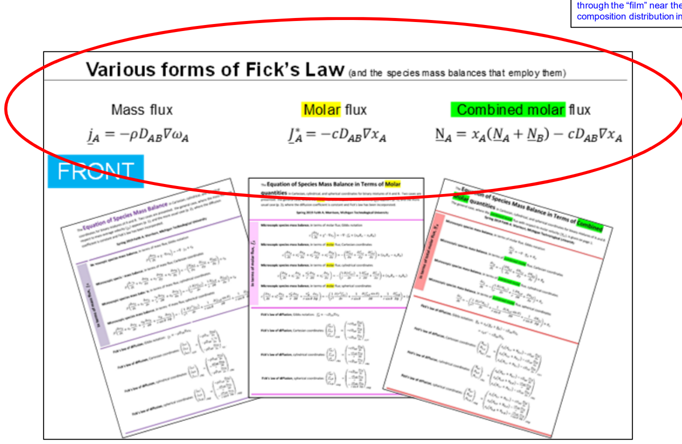
1D Steady Diffusion—Heterogeneous Chemical Reaction



Which approach is best for solving the model?



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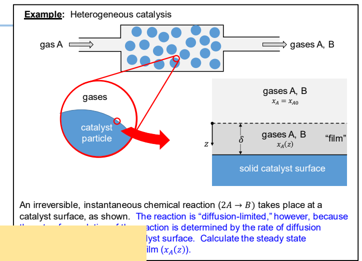
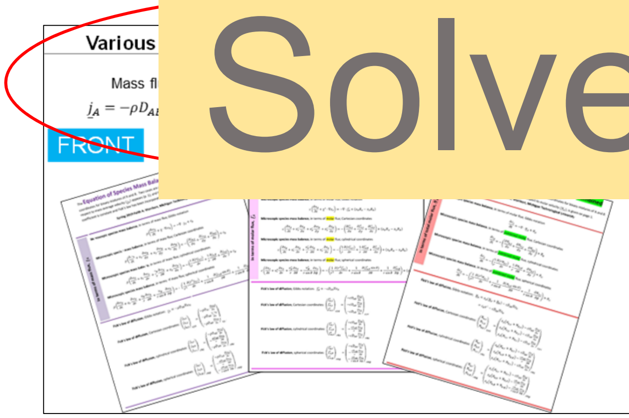
1D Steady Diffusion—Heterogeneous Chemical Reaction

Which approach is best for solving the model?





Solve

BSL2, p552

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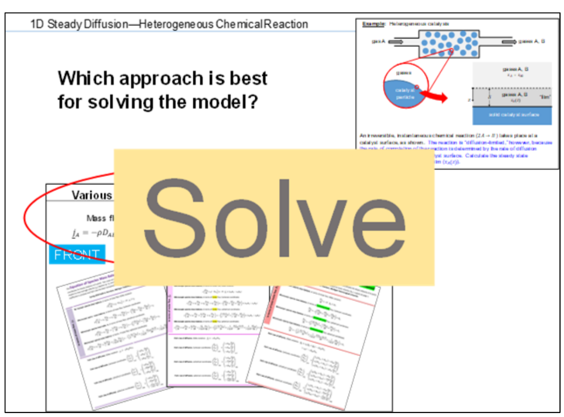
See hand notes for the start (Example 3)
Solution assigned in HW4a



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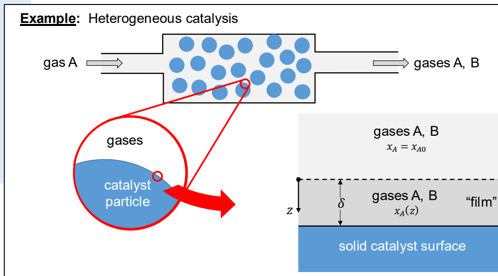
1D Steady Diffusion—Heterogeneous Chemical Reaction

Problem Summary: Heterogeneous Chemical Reaction

- One-dimensional (1D)
- Steady
- Use molar flux (due to reaction)
- Use combined molar flux $\underline{N}_A$; we can draw modeling simplifications about $\underline{N}_B$ due to *fast reaction*)
- Needed stoichiometry
- Boundary conditions: concentrations known (fast reaction ⇒ A disappears at surface.

Example: Heterogeneous catalysis



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

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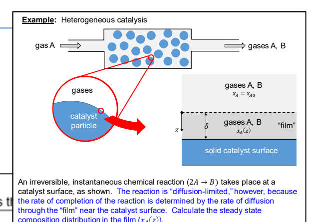
1D Steady Diffusion—Heterogeneous Chemical Reaction

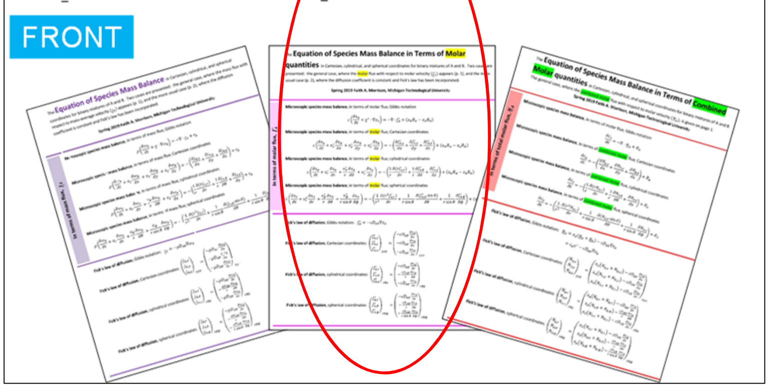
Could we have used $\underline{J}_A^*$ instead?



Various forms of Fick's Law (and the species mass balances t...

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

FRONT



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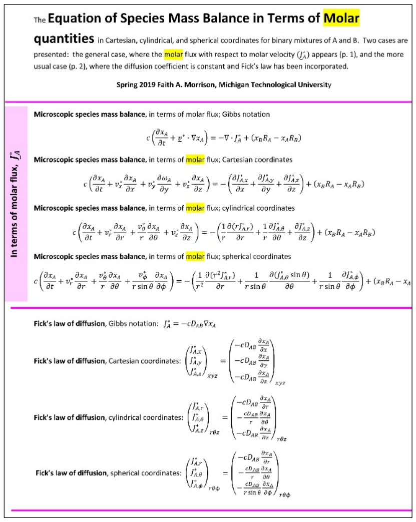
1D Steady Diffusion—Heterogeneous Chemical Reaction



$\underline{J}_A^*$: **Molar flux relative to a mixture's molar average velocity $\underline{v}^*$**

Definition:

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

Fick's law:

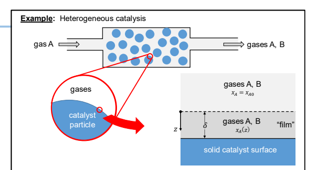
$$\underline{J}_A^* = -cD_{AB}\nabla x_A$$

Microscopic species A mass balance:

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

$R_A \equiv$ rate of production of moles of A by homogeneous chemical reaction per volume

1D Steady Diffusion—Heterogeneous Chemical Reaction



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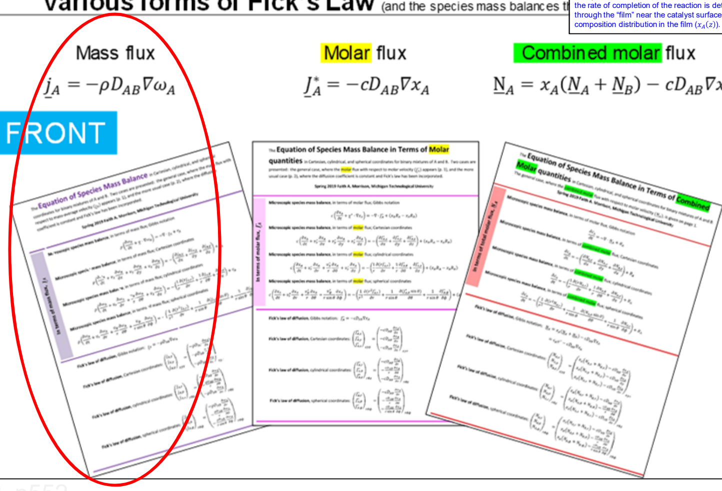
Could we have used $\underline{j}_A$ instead?

Various forms of Fick's Law (and the species mass balances th…

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



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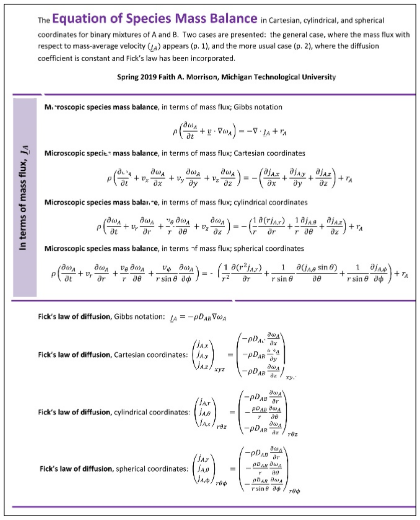
1D Steady Diffusion—Heterogeneous Chemical Reaction



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.

Spring 2019 Faith A. Morrison, Michigan Technological University

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

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

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

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

$$\rho\left(\frac{\partial \omega_A}{\partial t} + v_x\frac{\partial \omega_A}{\partial x} + v_y\frac{\partial \omega_A}{\partial y} + v_z\frac{\partial \omega_A}{\partial z}\right) = -\left(\frac{\partial j_{A,x}}{\partial x} + \frac{\partial j_{A,y}}{\partial y} + \frac{\partial j_{A,z}}{\partial z}\right) + r_A$$

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

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

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

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

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

Fick's law of diffusion, Cartesian coordinates: $\begin{pmatrix} j_{A,x} \\ j_{A,y} \\ j_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} -\rho D_{AB}\frac{\partial \omega_A}{\partial x} \\ -\rho D_{AB}\frac{\partial \omega_A}{\partial y} \\ -\rho D_{AB}\frac{\partial \omega_A}{\partial z} \end{pmatrix}_{xyz}$

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

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

$\underline{j}_A$: **Mass flux** relative to a **mixture's mass** average velocity $\underline{v}$

Definition:

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

Fick's law:

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

Microscopic species A mass balance:

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

$r_A \equiv$ rate of production of mass of A by homogeneous chemical reaction per volume

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1D Steady Diffusion—Heterogeneous Chemical Reaction

Problem Summary: Heterogeneous Chemical Reaction

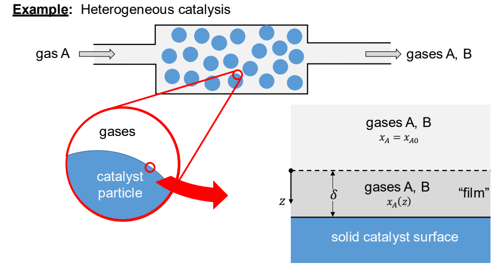
- One-dimensional (1D)
- Steady
- Use molar flux (due to reaction)
- Use combined molar flux $\underline{N}_A$; we can draw modeling simplifications about $\underline{N}_B$ due to fast reaction)
- Needed stoichiometry
- Boundary conditions: concentrations known (fast reaction ⇒ A disappears at surface.

Flux choice

Choose:

- **Molar** because there is a reaction
- **Combined molar** because the convection is only due to diffusion

Example: Heterogeneous catalysis



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

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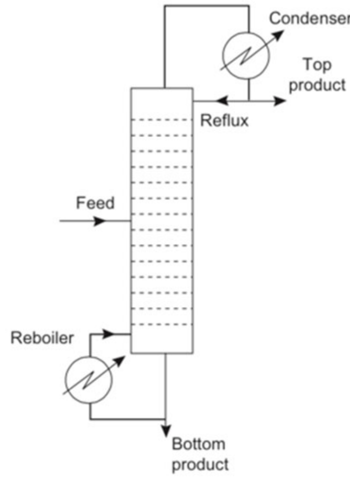
1D Steady Diffusion—Equimolar Counter Diffusion

Example: Mass transfer in Distillation

Image source: https://www.indiamart.com/proddetail/distillation-column-11044625255.html



https://processdesign.mccormick.northwestern.edu/index.php/Column

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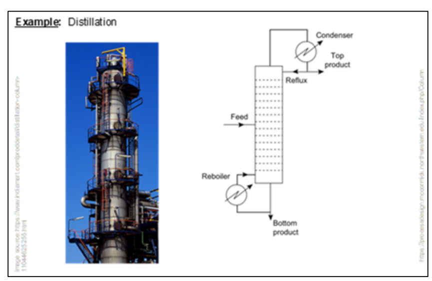
1D Steady Diffusion—Equimolar Counter Diffusion

Example: Distillation *(continued)*

In general, the molar flow rates in the enriching (L, V) and stripping $(\bar{L}, \bar{V})$ sections are not equal.

This is only true if every time a mole of vapor is condensed, a mole of liquid is vaporized (*Constant Molal Overflow*)



Constant Molal Overflow (CMO)

1. The heat of vaporization per mole λ is constant (independent of concentration)
2. Specific heat changes are small compared to latent heat changes
3. The column is adiabatic
4. The saturated liquid and vapor lines on an enthalpy-composition diagram (in molar units) are parallel

Wankat, pp110-1

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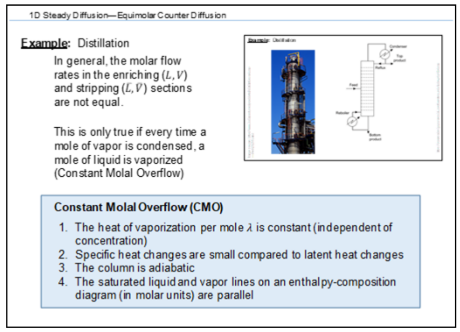
1D Steady Diffusion—Equimolar Counter Diffusion

Example: Distillation *(continued)*

"This is only true if every time a mole of vapor is condensed, a mole of liquid is vaporized (Constant Molal Overflow)"

This condition is met by equimolar counter diffusion.



1D Steady Diffusion—Equimolar Counter Diffusion

Example: Distillation

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Constant Molal Overflow (CMO)

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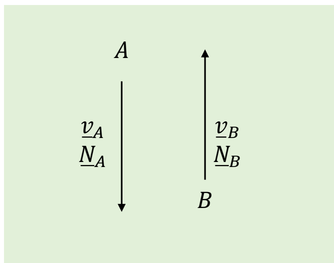


$$\underline{v}_A = -\underline{v}_B$$

$$\underline{N}_A = -\underline{N}_B$$

Note:

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

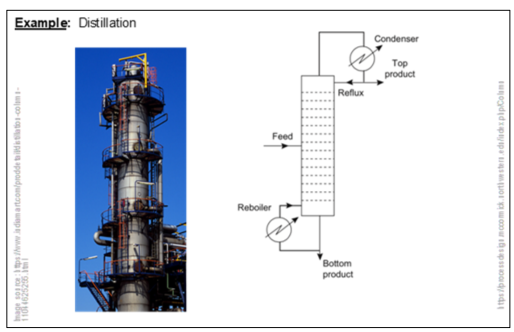
$$\Rightarrow \underline{v}^* = 0$$

WRF, p499

1D Steady Diffusion—Equimolar Counter Diffusion

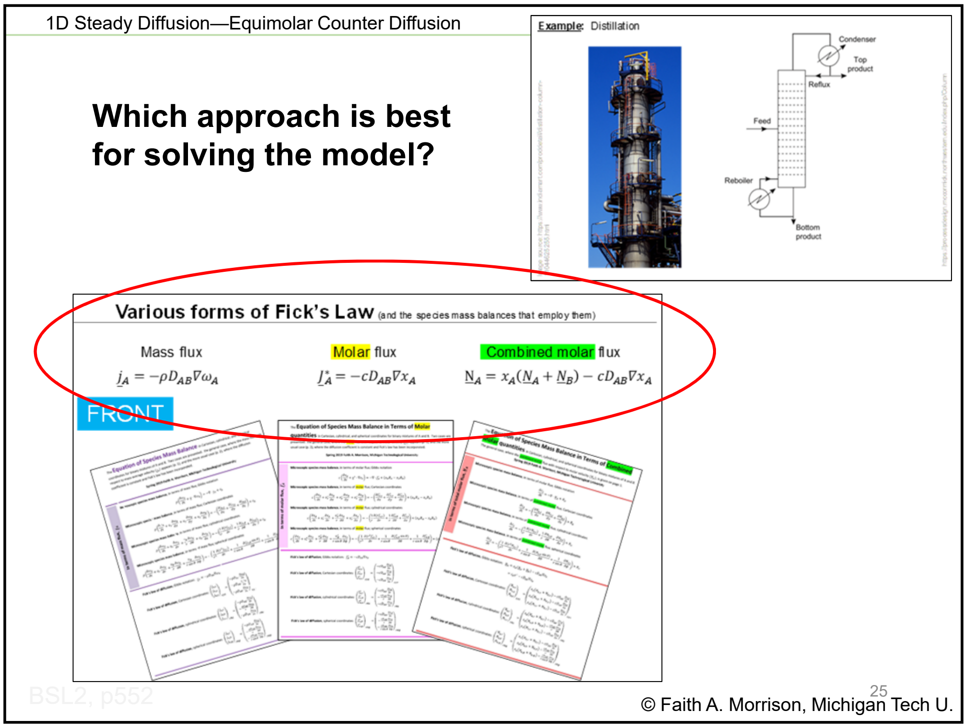
Example: Mass transfer in distillation *(continued)*

Equimolar Counter Diffusion



A distillation column is separating two components A and B at steady state. In the vapor phase the two components are moving in equimolar counter diffusion. What are the molar fluxes of A and B? What is the concentration distribution in the region of the equimolar counter diffuson?

Wankat, pp110-1


1D Steady Diffusion—Equimolar Counter Diffusion
Which approach is best for solving the model?
Example: Distillation
Condenser
Top product
Reflux
Feed
Reboiler
Bottom product
Various forms of Fick's Law (and the species mass balances that employ them)
Mass flux
$\underline{j}_A = -\rho D_{AB} \nabla \omega_A$
Molar flux
$\underline{J}_A^* = -c D_{AB} \nabla x_A$
Combined molar flux
$\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - c D_{AB} \nabla x_A$
FRONT
BSL2, p552
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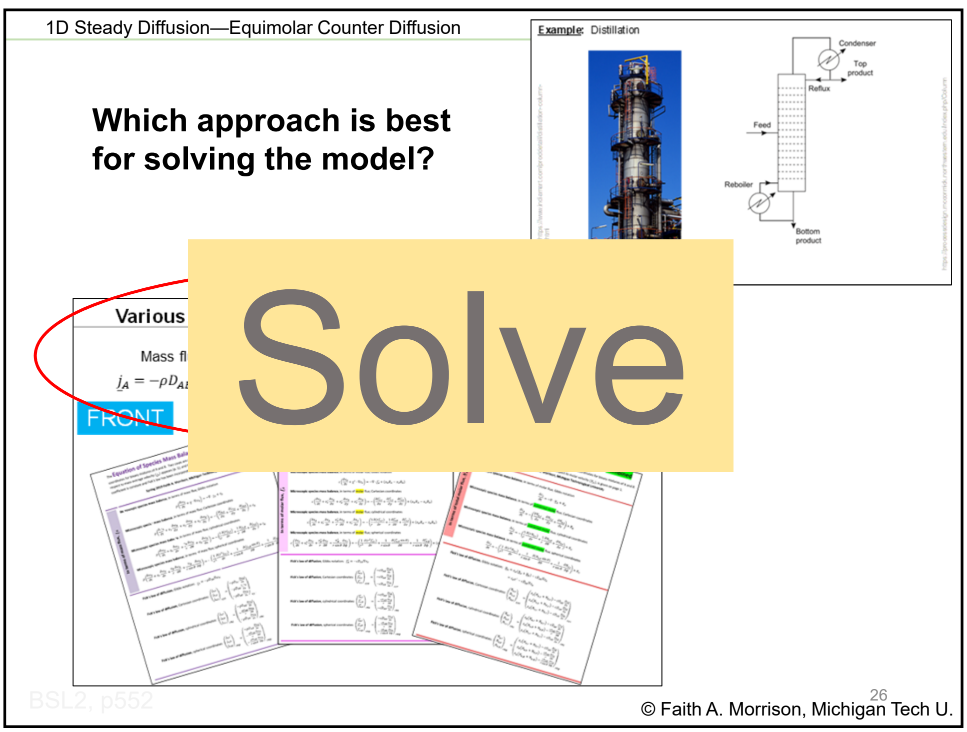
1D Steady Diffusion—Equimolar Counter Diffusion
Which approach is best for solving the model?
Example: Distillation
Condenser
Top product
Reflux
Feed
Reboiler
Bottom product
Solve
FRONT
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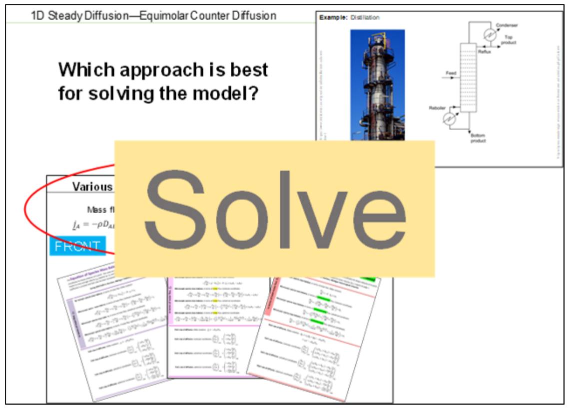
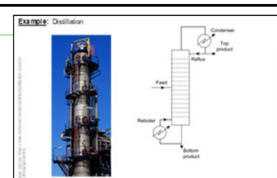
See hand notes for the start (Example 4)
Solution assigned in HW4a



1D Steady Diffusion—Equimolar Counter Diffusion

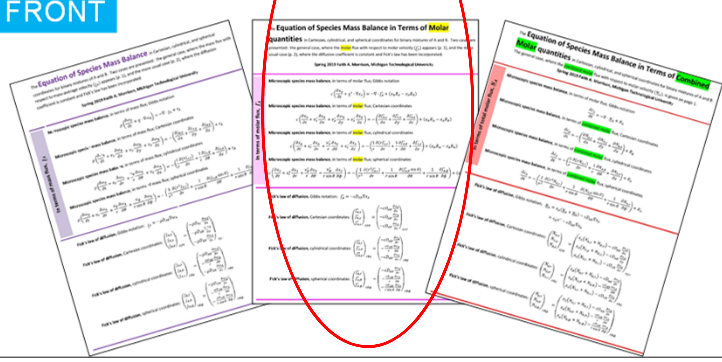


Could we have used $\underline{J}_A^*$ instead?

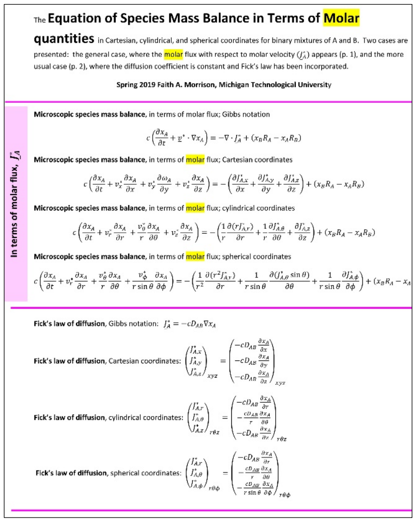
Various forms of Fick's Law (and the species mass balances that employ them)

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

FRONT



1D Steady Diffusion—Equimolar Counter Diffusion



$\underline{J}_A^*$: **Molar flux** relative to a **mixture's molar** average velocity $\underline{v}^*$

Definition:

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

Fick's law:

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

Microscopic species A mass balance:

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

$R_A \equiv$ rate of production of moles of A by **homogeneous** chemical reaction per volume

(The two fluxes are the same for equimolar counter diffusion)

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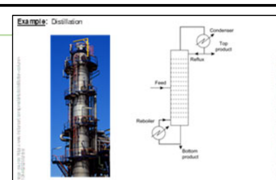
1D Steady Diffusion—Equimolar Counter Diffusion

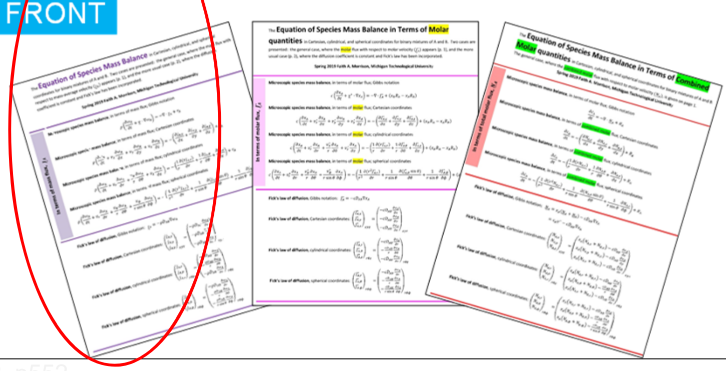


Could we have used $\underline{j}_A$ instead?

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



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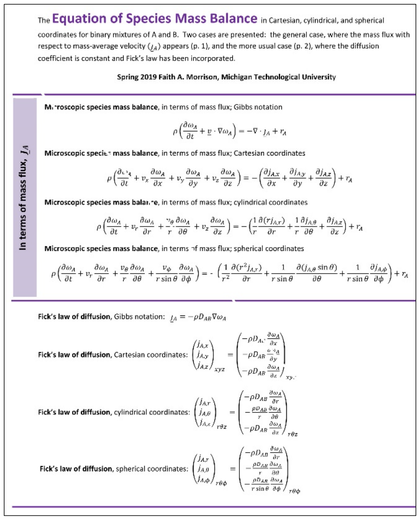
1D Steady Diffusion—Equimolar Counter Diffusion



The **Equation of Species Mass Balance** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. Two cases are presented: the general case, where the mass flux with respect to mass-average velocity ($\underline{j}_A$) appears (p. 1), and the more usual case (p. 2), where the diffusion coefficient is constant and Fick's law has been incorporated.

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

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

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

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

$$\rho\left(\frac{\partial \omega_A}{\partial t} + v_x\frac{\partial \omega_A}{\partial x} + v_y\frac{\partial \omega_A}{\partial y} + v_z\frac{\partial \omega_A}{\partial z}\right) = -\left(\frac{\partial j_{A,x}}{\partial x} + \frac{\partial j_{A,y}}{\partial y} + \frac{\partial j_{A,z}}{\partial z}\right) + r_A$$

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

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

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

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

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

Fick's law of diffusion, Cartesian coordinates: $\begin{pmatrix} j_{A,x} \\ j_{A,y} \\ j_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} -\rho D_{AB}\frac{\partial \omega_A}{\partial x} \\ -\rho D_{AB}\frac{\partial \omega_A}{\partial y} \\ -\rho D_{AB}\frac{\partial \omega_A}{\partial z} \end{pmatrix}_{xyz}$

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

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

$\underline{j}_A$: **Mass flux relative to a mixture's mass average velocity** $\underline{v}$

Definition:

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

Fick's law:

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

Microscopic species A mass balance:

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

(there is no advantage to the mass perspective in this case)

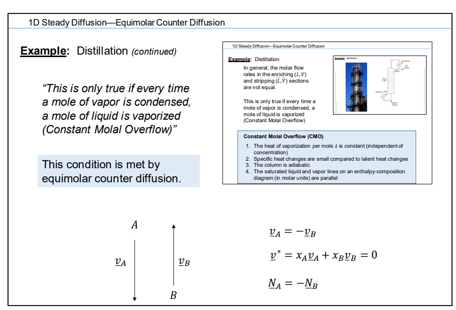
$r_A \equiv$ rate of production of mass of A by **homogeneous** chemical reaction per volume

1D Steady Diffusion—Equimolar Counter Diffusion

Problem Summary: Equimolar Counter Diffusion

- One-dimensional (1D)
- Steady
- Use molar flux (due to equimolar counter diffusion specified)
- Use combined molar flux $\underline{N}_A$ or $\underline{J}_A^*$)
- Boundary conditions: concentrations known over a known distance

Flux choice
Choose:
- **Molar** because equi*molar* motion was specified
- **Combined molar** and **molar** are the same when $\underline{v}^* = 0$ ($\underline{N}_A = \underline{J}_A^*$)



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

These two molar fluxes are the same when $\underline{v}^* = 0$.

1D Steady Diffusion

Problems Summary

1. Unimolecular mass transfer (evaporating tank, Ex 1)

✓ 2. Heterogeneous chemical reaction (catalytic converter, Ex 3, convection only due to diffusion)

✓ 3. Equimolar counter diffusion (distillation, $\underline{v}^* = 0, (\underline{N}_A = \underline{J}_A^*)$ Ex 4)

4. Homogeneous chemical reaction

1D Steady Diffusion

Problems Summary

We did this earlier →

Could we have taken a different approach?

1. Unimolecular mass transfer (evaporating tank, Ex 1)

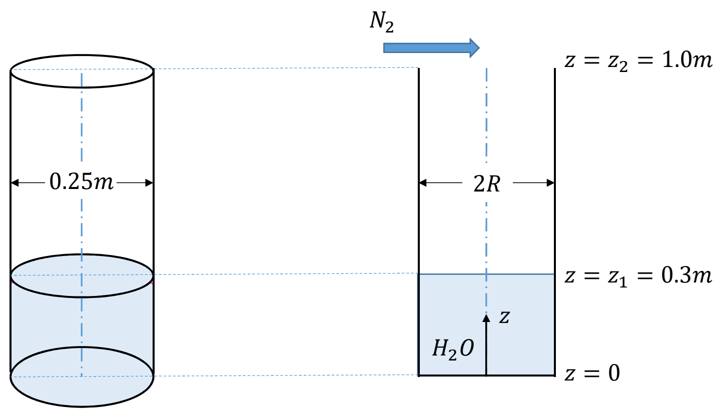
✓ 2. Heterogeneous chemical reaction (catalytic converter, Ex 3, convection only due to diffusion)

✓ 3. Equimolar counter diffusion (distillation, $\underline{v}^* = 0, (\underline{N}_A = \underline{J}_A^*)$ Ex 4)

4. Homogeneous chemical reaction

1D Steady Diffusion—Unimolecular MassTransfer (film theory)

Example: Water $(40^oC, 1.0\ atm)$ slowly and steadily evaporates into nitrogen $(40^oC, 1.0\ atm)$ 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. **What is the rate of water evaporation?**



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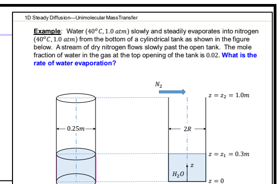
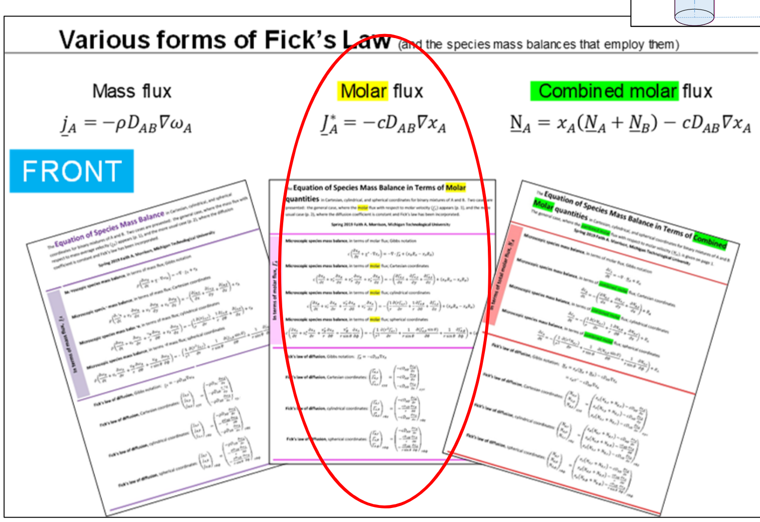
1D Steady Diffusion—Unimolecular MassTransfer (film theory)



Could we have used $\underline{J}_A^*$ instead?



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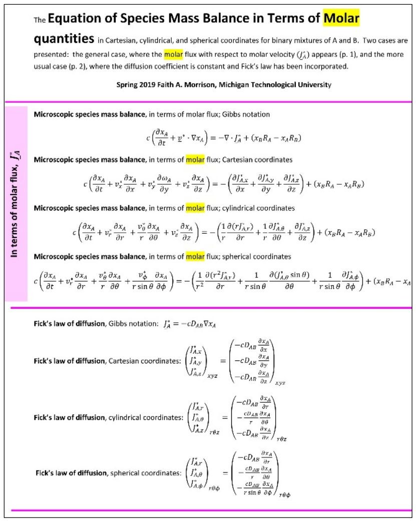
1D Steady Diffusion—Unimolecular MassTransfer (film theory)



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.

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

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

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

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

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

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

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

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

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

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: $\begin{pmatrix}J_{A,r}^*\\J_{A,\theta}^*\\J_{A,\phi}^*\end{pmatrix}_{r\theta\phi}=\begin{pmatrix}-cD_{AB}\frac{\partial x_A}{\partial r}\\-\frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta}\\-\frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi}\end{pmatrix}_{r\theta\phi}$

$\underline{J}_A^*$: **Molar flux relative to a mixture's molar average velocity $\underline{v}^*$**

Definition:

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

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Microscopic species A mass balance:

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

(Let's explore $\underline{v}^*$ in some limits)

$R_A\equiv$ rate of production of moles of A by homogeneous chemical reaction per volume

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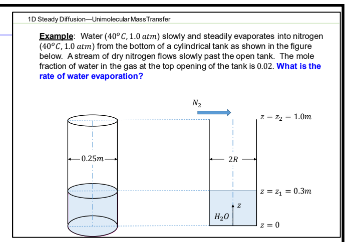
1D Steady Diffusion—Unimolecular MassTransfer (film theory)



Could we have used $\underline{J}_A^*$ instead of $\underline{N}_A$?

Definition:

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

Definition:

$$\underline{N}_A=cx_A\underline{v}_A$$

When is $\underline{v}^*=0$?

B is stagnant $\Rightarrow \underline{v}_B=0$.

If A is dilute, $x_A\approx 0$

then, $\underline{v}^*\approx 0$.

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

$$=x_A\underline{v}_A$$

Stagnant B, dilute A

$\underline{v}^*\approx 0$

$\underline{J}_A^*=\underline{N}_A$

$\underline{J}_A^*$ and $\underline{N}_A$ are equal for stagnant B, dilute A

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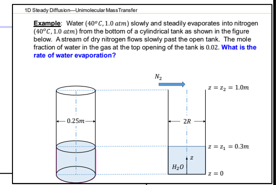
1D Steady Diffusion—Unimolecular MassTransfer (film theory)

Could we have used $\underline{j}_A$ instead?



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

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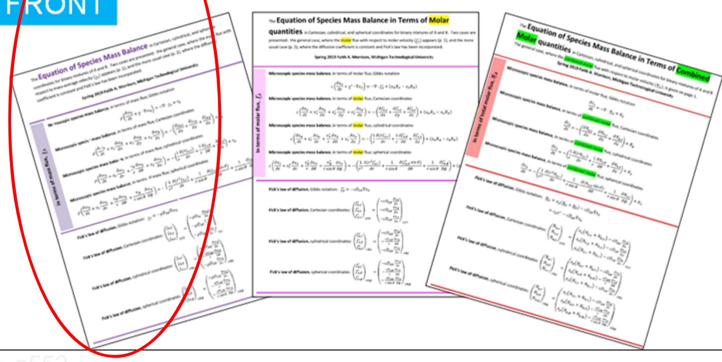

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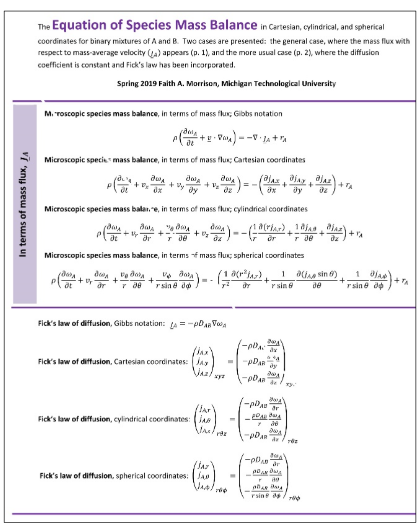
1D Steady Diffusion—Unimolecular MassTransfer (film theory)



The **Equation of Species Mass Balance** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. Two cases are presented: the general case, where the mass flux with respect to mass-average velocity ($\underline{j}_A$) appears (p. 1), and the more usual case (p. 2), where the diffusion coefficient is constant and Fick's law has been incorporated.

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

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

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

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

$$\rho\left(\frac{\partial\omega_A}{\partial t} + v_x\frac{\partial\omega_A}{\partial x} + v_y\frac{\partial\omega_A}{\partial y} + v_z\frac{\partial\omega_A}{\partial z}\right) = -\left(\frac{\partial j_{A,x}}{\partial x} + \frac{\partial j_{A,y}}{\partial y} + \frac{\partial j_{A,z}}{\partial z}\right) + r_A$$

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

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

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

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

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Fick's law of diffusion, Cartesian coordinates: $\begin{pmatrix} j_{A,x} \\ j_{A,y} \\ j_{A,z}\end{pmatrix}_{xyz} = \begin{pmatrix} -\rho D_{AB}\frac{\partial\omega_A}{\partial x} \\ -\rho D_{AB}\frac{\partial\omega_A}{\partial y} \\ -\rho D_{AB}\frac{\partial\omega_A}{\partial z}\end{pmatrix}_{xyz}$

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

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

$\underline{j}_A$: Mass flux relative to a mixture's mass average velocity $\underline{v}$

Definition:

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Fick's law:

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

Microscopic species A mass balance:

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

$r_A \equiv$ rate of production of mass of A by homogeneous chemical reaction per volume

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1D Steady Diffusion—Unimolecular MassTransfer (film theory)

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

$$\rho\left(\frac{\partial \omega_A}{\partial t} + v_x\frac{\partial \omega_A}{\partial x} + v_y\frac{\partial \omega_A}{\partial y} + v_z\frac{\partial \omega_A}{\partial z}\right) = -\left(\frac{\partial j_{A,x}}{\partial x} + \frac{\partial j_{A,y}}{\partial y} + \frac{\partial j_{A,z}}{\partial z}\right) + r_A$$

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

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

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

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

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

Fick's law of diffusion, Cartesian coordinates: $\begin{pmatrix} j_{A,x} \\ j_{A,y} \\ j_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} -\rho D_{AB}\frac{\partial \omega_A}{\partial x} \\ -\rho D_{AB}\frac{\partial \omega_A}{\partial y} \\ -\rho D_{AB}\frac{\partial \omega_A}{\partial z} \end{pmatrix}_{xyz}$

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

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

$\underline{j}_A$: **Mass flux** relative to a **mixture's mass** average velocity $\underline{v}$

Definition:

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

Fick's law:

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

Microscopic species A mass balance:

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

(There is no advantage to the mass perspective in this case)

$r_A \equiv$ rate of production of mass of A by homogeneous chemical reaction per volume

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1D Steady Diffusion—Unimolecular MassTransfer (film theory)

Problem Summary: Unimolecular Mass Transfer (film theory)

- One-dimensional (1D)
- Steady
- Use molar flux
- Use combined molar flux $\underline{N}_A$
- Boundary conditions: concentrations known over a known distance

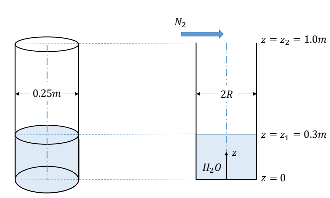
Flux choice

Choose:

- **Molar** because mole fractions specified
- **Combined molar** and **molar** are the same when **B is *stagnant and A is dilute*** (implies $\underline{v}^* = 0$)

1D Steady Diffusion—Unimolecular MassTransfer

Example: Water ($40^oC, 1.0\ atm$) slowly and steadily evaporates into nitrogen ($40^oC, 1.0\ atm$) 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. **What is the rate of water evaporation?**



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

These two molar fluxes are the same when $\underline{v}^* = 0$.

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Problems Summary

✓ 1. Unimolecular mass transfer (evaporating tank, Ex 1; evaporating droplet, Ex 2)
   - Subcase: stagnant B, dilute A, $\underline{v}^* \approx 0, \Rightarrow \underline{\mathrm{N}}_{\mathrm{A}} = \underline{\mathrm{J}}_{\mathrm{A}}^*$

✓ 2. Heterogeneous chemical reaction (catalytic converter, Ex 3, convection only due to diffusion)

✓ 3. Equimolar counter diffusion (distillation, $\underline{v}^* = 0, (\underline{N}_A = \underline{J}_A^*)$ Ex 4)

→ 4. Homogeneous chemical reaction

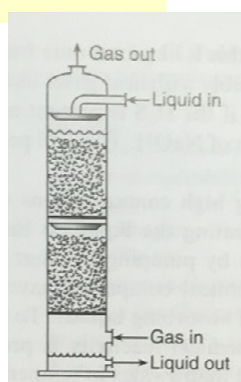
End lecture 7

Gas Absorption

Image source: www.sulzer.com

While a chemical plant would not exist without the chemical reactors, the biggest expense (the biggest equipment) will often be the separation equipment, **distillation columns** and **gas absorption columns**.

- Packed column (tower)
- Liquid poured into top trickles down through packing
- Gas pumped into bottom flows upward
- Analysis involves both **fluid mechanics** (determines cross-sectional area) and **mass transfer** (determines height)

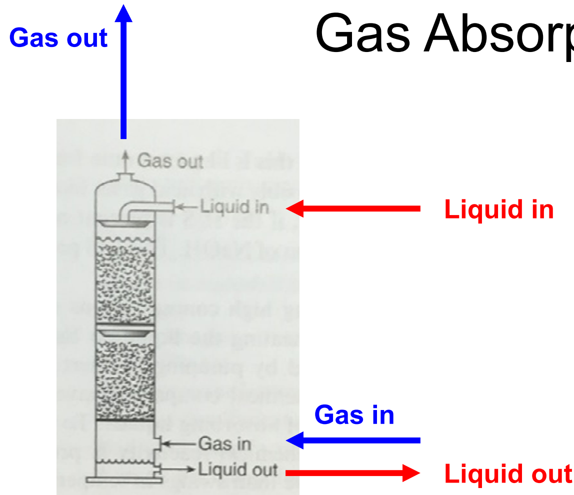


Begin lecture 8

Cussler, p305, 7

1D Steady Diffusion—Gas Absorption with Chemical Solvent

Gas Absorption



Exiting liquid stream contains high concentrations of the impurity. This is later "stripped" by heating the liquid so that the impurity bubbles out.

The "swing" in temperature may sometimes be replaced by a "swing" in pressure (lowers costs)

Cussler, p307

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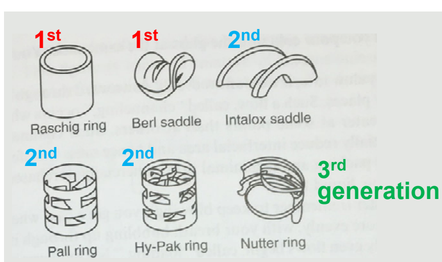
1D Steady Diffusion—Gas Absorption with Chemical Solvent

Designed by 80 years of experience

Gas Absorption Packing

High fluid flow trades off with high interfacial area (both are desired)



6 types of random packing; cheaper, common

Image source: www.sulzer.com

Structured packing; pricey, more efficient (up to 30% more efficient); fluids move past each other with less bypassing

Cussler, p308,9

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Gas Absorption-the liquids

What are the gases to be absorbed?
*What are the **liquids** that absorb them?*

Some depend on the solubility of the gas
Most react chemically with the components of the gas

Choice depends on the concentrations in the feed gas mixture and on the desired percent removal

High concentration (10-50%): dissolve in a nonvolatile, nonreactive liquid, aka **physical solvent** *(less common, but simpler)*

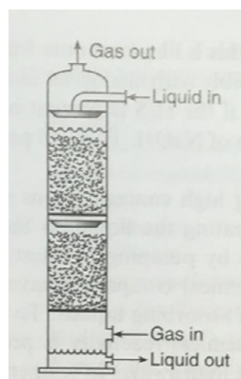
Lower concentration (1-10%): use liquid capable of fast, reversible chemical reaction with the gas to be removed, aka **chemical solvent** *(20X more common, but complex)*

Very low concentration (<1%): use an adsorbent that reacts irreversibly (this is expensive; may produce solid waste).

Cussler, p306,7

Gas Absorption Tower Design

A type of "differential contacting"



Design: Diameter, Height

Diameter: constrained by the fluid mechanics of the gas and liquid flowing past each other; complicated; described by largely empirical correlations (use turnkey procedure)

Height: must be sufficient to attain the separation desired; depends on how solubility depends on concentration (linear or nonlinear isotherm, dilute (easy), not dilute (hard))

Cussler, p304

Gas Absorption

Gas Absorption Tower Design

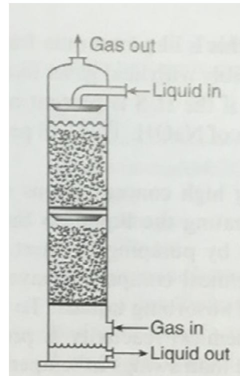
A type of "differential contacting"

Design: Diameter, Height

Complicated; solved by trial and error

- Diameter: constrained by the fluid mechanics of the gas and liquid flowing past each other; complicated; described by largely empirical correlations (use turnkey procedure)
- Height: must be sufficient to attain the separation desired; depends on how solubility depends on concentration (linear or nonlinear isotherm, dilute (easy), not dilute (hard))

Can be modeled.



Cussler, p304

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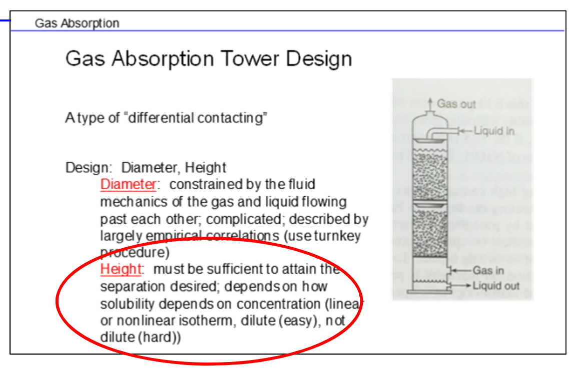
1D Steady Diffusion—Gas Absorption

Column height must be sufficient to attain the separation desired.



We need a *model* of how the separation is achieved to produce the design equations for the height of the column.

A model that **works** will reveal what the physics of the unit is.

Models that **only partially work** also reveal important aspects of the physics.

Cussler, p304

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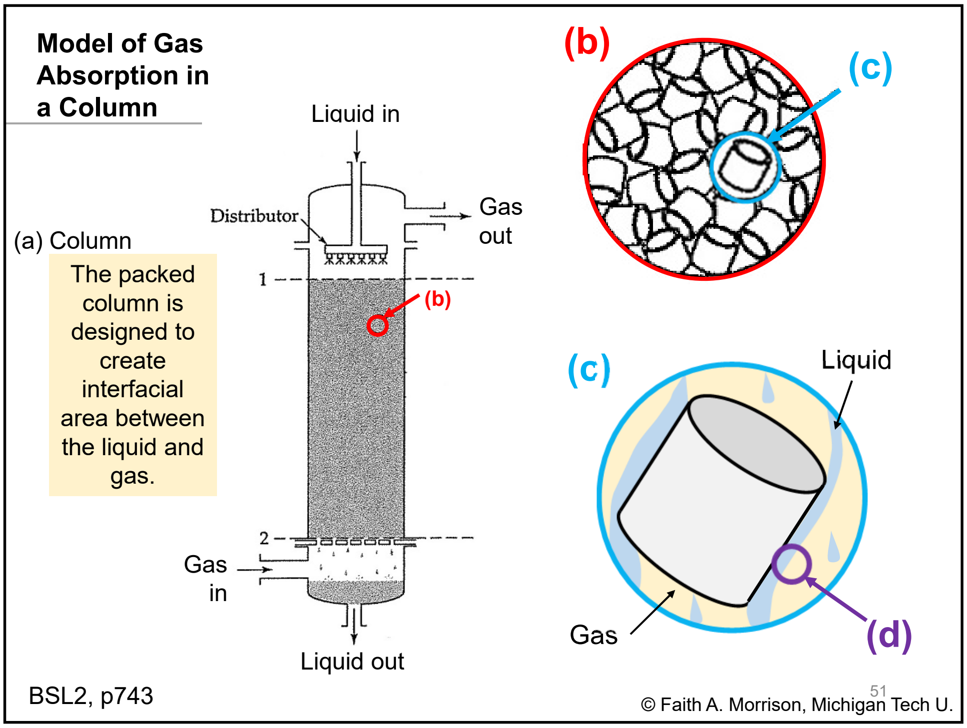


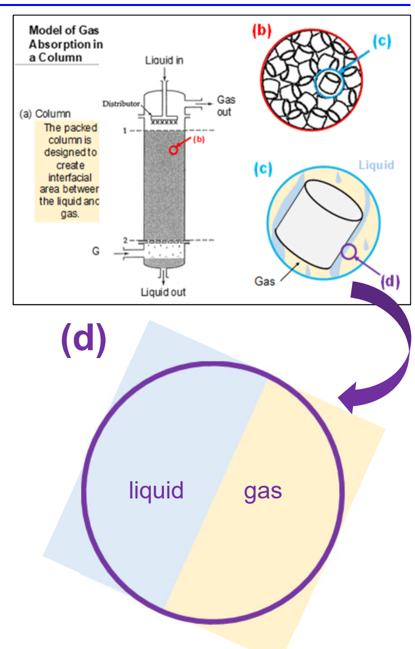
1D Steady Diffusion—Gas Absorption with Chemical Solvent

The Mass-Transfer Model

We focus on the **liquid-gas interface** where the mass transfer takes place.

Idealize the **entire device** as comprising only the appropriate amount of this interface, with mass transfer taking place.

Retain the role of the column, by forcing the appropriate concentrations of species A enter and exit the column.



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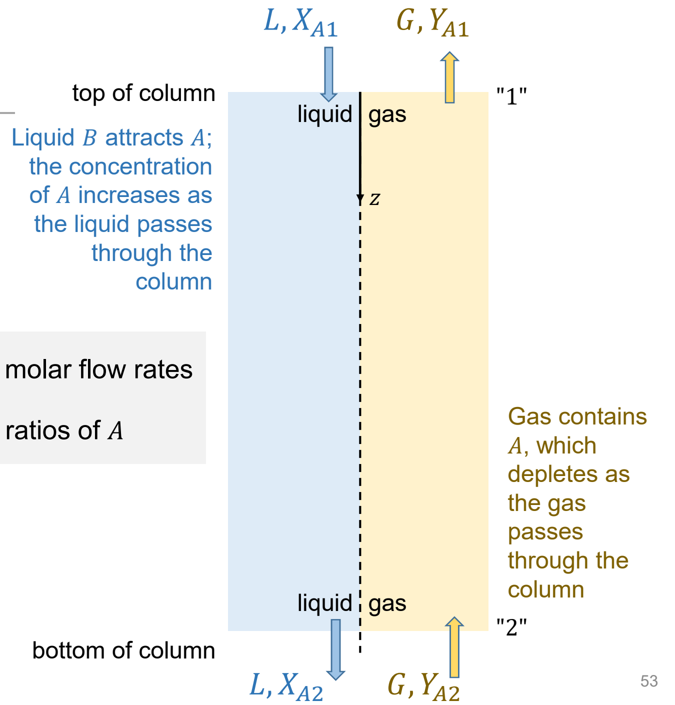
Model of Gas Absorption in a Column



L, G	A-free molar flow rates
X_{A1}, Y_{A1}	Molar ratios of A

BSL2, p742

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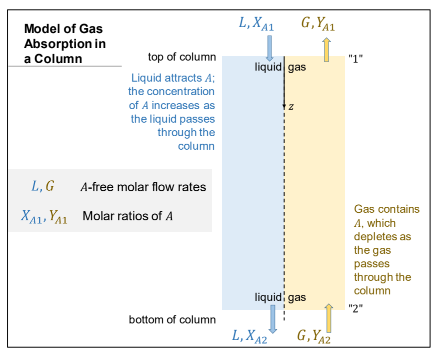
1D Steady Diffusion—Gas Absorption with Chemical Solvent

Example: Mass transfer a Gas Absorption Column (Chemical Solvent)



A gas absorption column is operating at steady state. The gas stream is composed of component A and an inert carrier gas I. The liquid stream is chemical absorbent B. Component A diffuses across the gas-liquid interface until it reacts with B. What are the molar fluxes of A and B? What is the concentration distribution in the region in which A diffuses into liquid B?

Wankat, pp110-1

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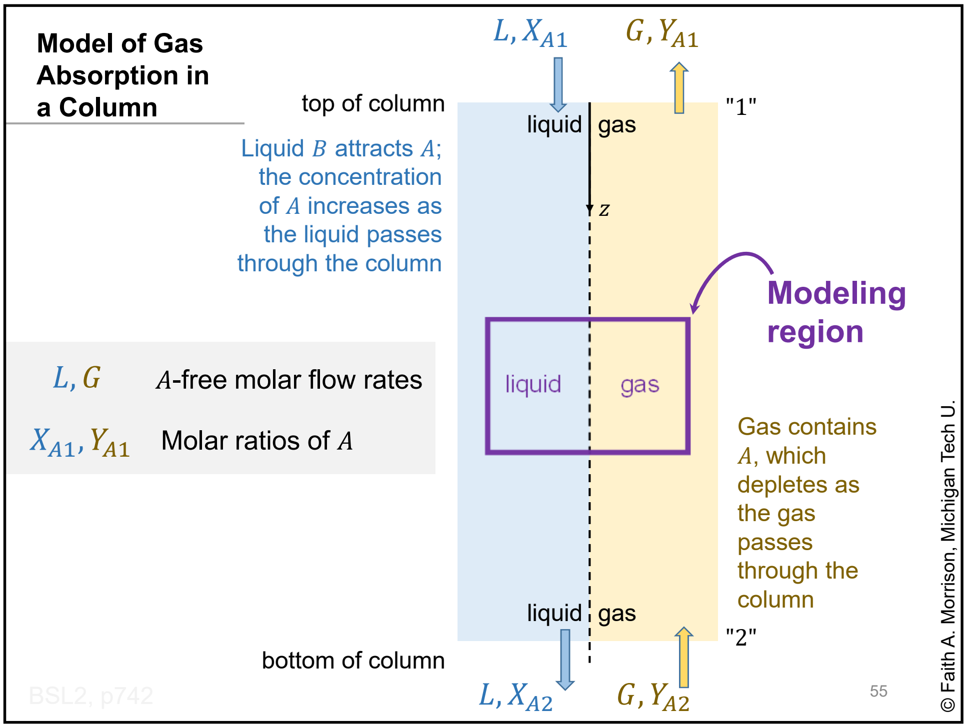
Model of Gas Absorption in a Column
L, X_{A1}
G, Y_{A1}
top of column
"1"
liquid
gas
Liquid B attracts A; the concentration of A increases as the liquid passes through the column
z
Modeling region
liquid
gas
L, G A-free molar flow rates
X_{A1}, Y_{A1} Molar ratios of A
Gas contains A, which depletes as the gas passes through the column
liquid
gas
"2"
bottom of column
L, X_{A2}
G, Y_{A2}
BSL2, p742
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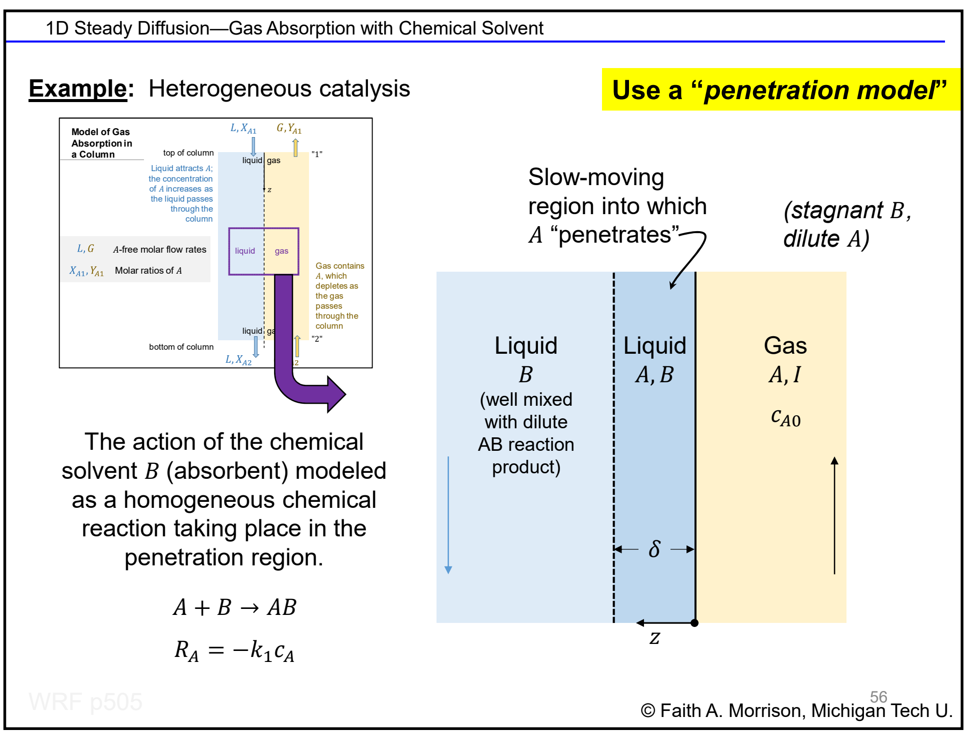
1D Steady Diffusion—Gas Absorption with Chemical Solvent
Example: Heterogeneous catalysis
Use a "penetration model"
Model of Gas Absorption in a Column
The action of the chemical solvent B (absorbent) modeled as a homogeneous chemical reaction taking place in the penetration region.
$A + B \rightarrow AB$
$R_A = -k_1 c_A$
Slow-moving region into which A "penetrates"
(stagnant B, dilute A)
Liquid
B
(well mixed with dilute AB reaction product)
Liquid
A, B
Gas
A, I
c_{A0}
δ
z
WRF p505
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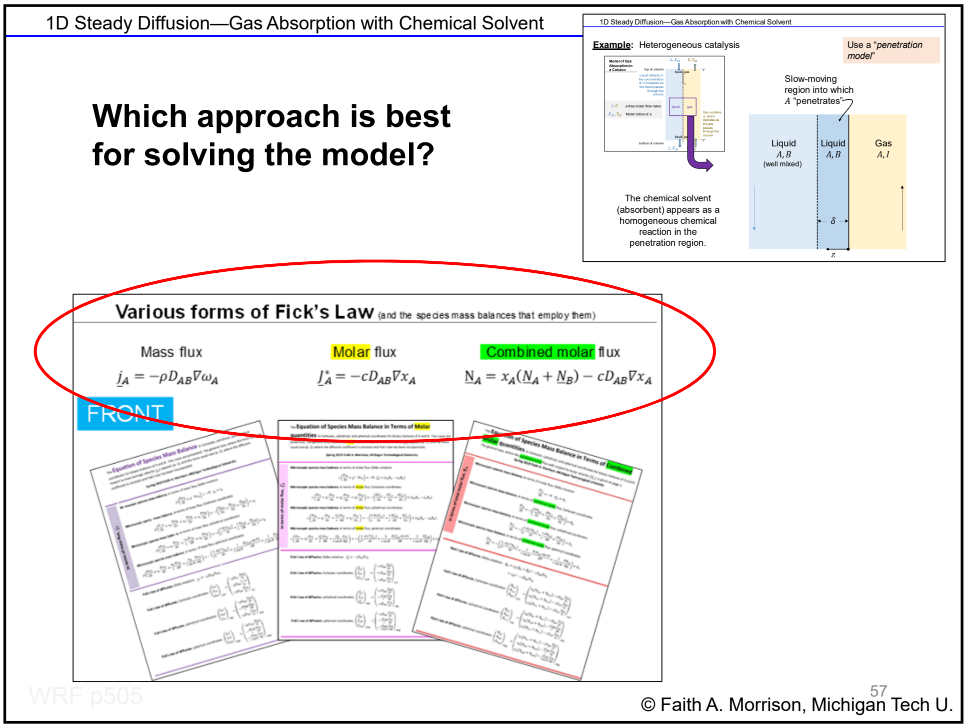
1D Steady Diffusion—Gas Absorption with Chemical Solvent
Which approach is best for solving the model?
Example: Heterogeneous catalysis
Use a "penetration model"
Slow-moving region into which A "penetrates"
Liquid A, B (well mixed)
Liquid A, B
Gas A, I
The chemical solvent (absorbent) appears as a homogeneous chemical reaction in the penetration region.
Various forms of Fick's Law (and the species mass balances that employ them)
Mass flux
$\underline{j}_A = -\rho D_{AB} \nabla \omega_A$
Molar flux
$\underline{J}_A^* = -c D_{AB} \nabla x_A$
Combined molar flux
$\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - c D_{AB} \nabla x_A$
FRONT
WRF p505
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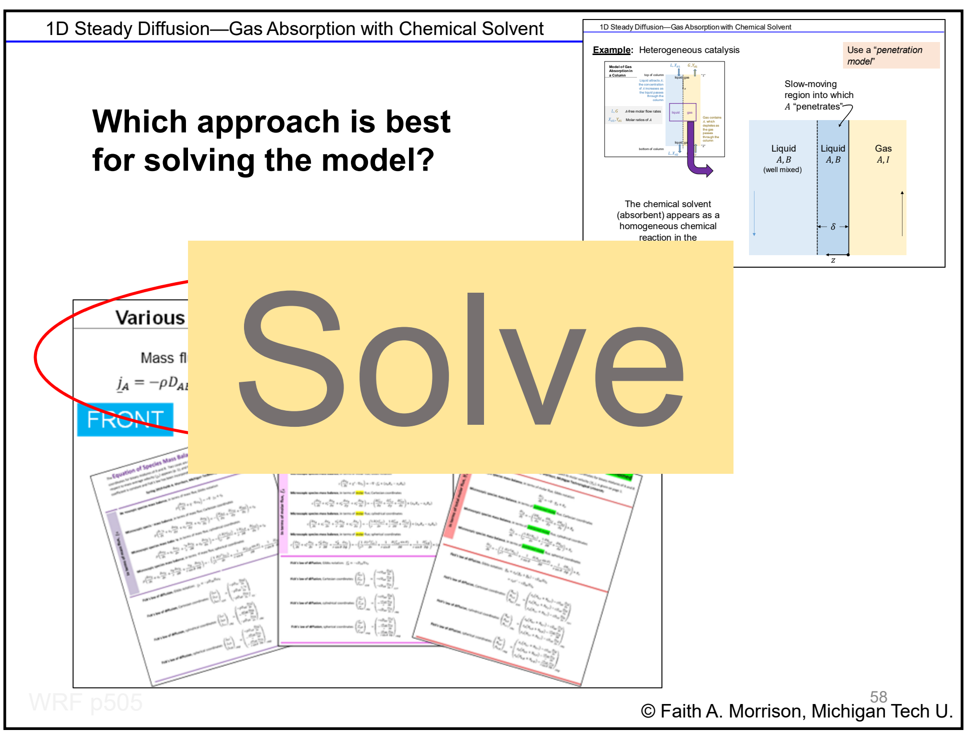
1D Steady Diffusion—Gas Absorption with Chemical Solvent
Which approach is best for solving the model?
Example: Heterogeneous catalysis
Use a "penetration model"
Slow-moving region into which A "penetrates"
Liquid A, B (well mixed)
Liquid A, B
Gas A, I
Solve
FRONT
WRF p505
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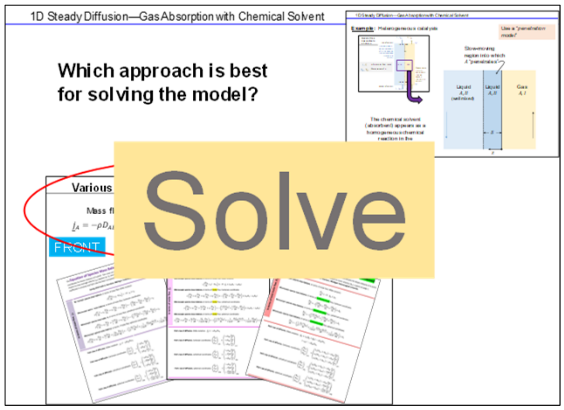
See hand notes for the start (Example 5)
Solution assigned in HW4a



BSL2, p552

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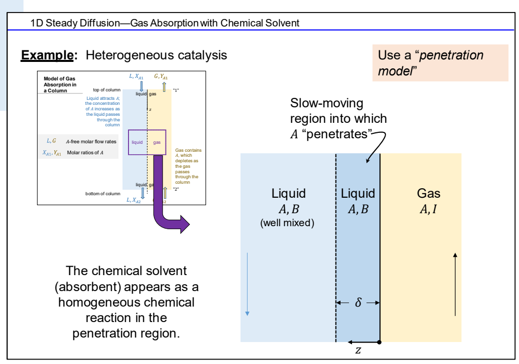
1D Steady Diffusion—Gas Absorption with Chemical Solvent

Problem Summary: Gas Absorption with Chemical Solvent

- One-dimensional (1D)
- Steady
- Use molar flux (due to reaction)
- Use combined molar flux $\underline{N}_A$)
- Needed stoichiometry and rate equation
- Boundary conditions: concentrations known (A disappears at penetration length)



WRF p505

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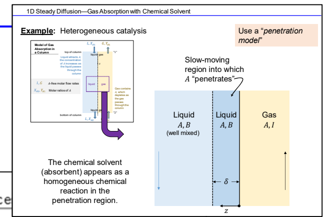
1D Steady Diffusion—Gas Absorption with Chemical Solvent

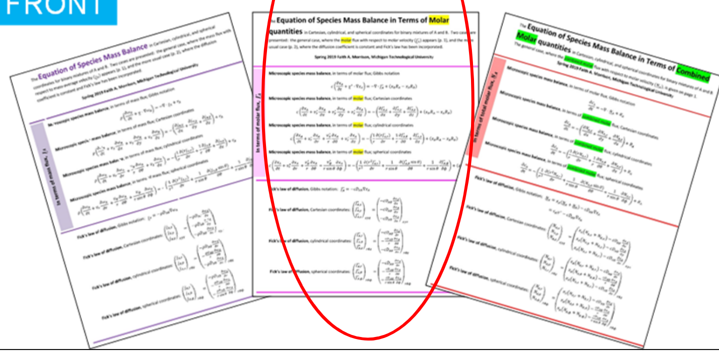
Could we have used $\underline{J}_A^*$ instead?



Various forms of Fick's Law (and the species mass balance)

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



WRF p505

1D Steady Diffusion—Gas Absorption with Chemical Solvent

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.

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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

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

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

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

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: $\begin{pmatrix} J_{A,r}^* \\ J_{A,\theta}^* \\ J_{A,\phi}^* \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} -cD_{AB}\frac{\partial x_A}{\partial r} \\ -\frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ -\frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$

$\underline{J}_A^*$: Molar flux relative to a mixture's molar average velocity $\underline{v}^*$

Definition:

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

Fick's law:

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

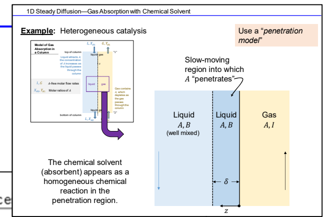
Microscopic species A mass balance:

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

$R_A \equiv$ rate of production of moles of A by homogeneous chemical reaction per volume

1D Steady Diffusion—Gas Absorption with Chemical Solvent

Could we have used $\underline{j}_A$ instead?



Various forms of Fick's Law (and the species mass balance)

Mass flux	Molar flux	Combined molar flux
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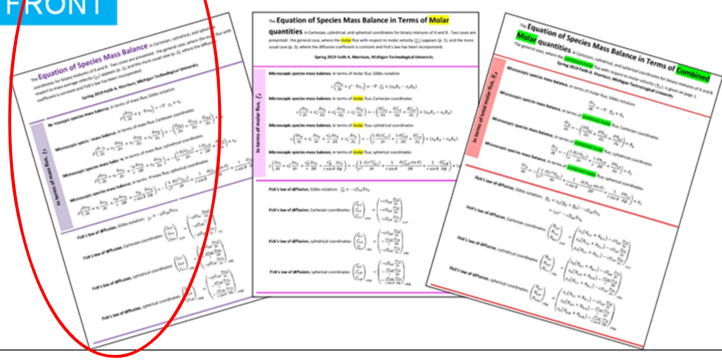
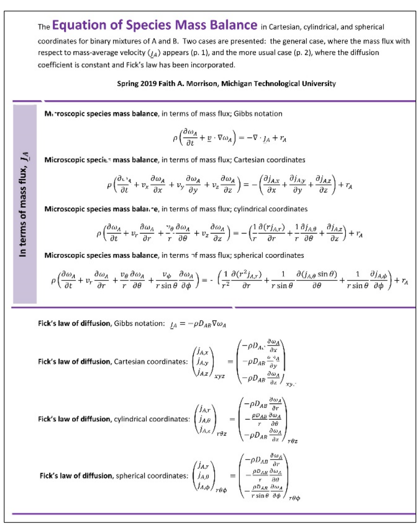


1D Steady Diffusion—Gas Absorption with Chemical Solvent



$\underline{j}_A$: **Mass flux relative to a mixture's mass average velocity $\underline{v}$**

Definition:

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Fick's law:

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

Microscopic species A mass balance:

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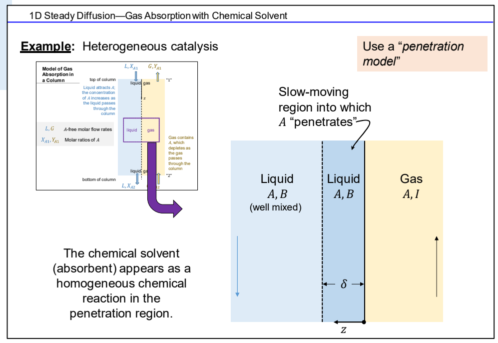
$r_A \equiv$ rate of production of mass of A by homogeneous chemical reaction per volume

1D Steady Diffusion—Gas Absorption with Chemical Solvent

Problem Summary: Gas Absorption with Chemical Solvent

- One-dimensional (1D)
- Steady
- Use molar flux (due to reaction)
- Use combined molar flux ($\underline{N}_A$)
- Needed stoichiometry and rate equation
- Boundary conditions: concentrations known (A disappears at penetration length)

Flux choice
Choose:
- **Molar** because there is a reaction
- **Combined molar** because the convection is only due to diffusion



1D Steady Diffusion

1D Steady Diffusion, Problems Summary

✓ 1. Unimolecular mass transfer (evaporating tank, Ex 1; evaporating droplet, Ex 2)
   - Subcase: stagnant B, dilute A, $\underline{v}^* \approx 0$, ($\underline{N}_A \approx \underline{J}_A^*$)

✓ 2. Heterogeneous chemical reaction (catalytic converter, Ex 3, convection only due to diffusion)

✓ 3. Equimolar counter diffusion (distillation, $\underline{v}^* = 0$, ($\underline{N}_A = \underline{J}_A^*$) Ex 4)

✓ 4. Homogeneous chemical reaction (gas absorption by chemical solvent, Ex 5, convection only due to diffusion)

1D Steady Diffusion

1D Steady Diffusion, Problems Summary

✓ 1. Unimolecular mass transfer (evaporating tank, Ex 1; evaporating droplet, Ex 2)
   - Subcase: stagnant B, dilute A, $\underline{v}^* \approx 0$, $(\underline{N}_A \approx \underline{J}_A^*)$

   ← *Film Model*

✓ 2. Heterogeneous chemical reaction (catalytic converter, Ex 3, convection only due to diffusion)

✓ 3. Equimolar counter diffusion (distillation, $\underline{v}^* = 0$, $(\underline{N}_A = \underline{J}_A^*)$ Ex 4)

✓ 4. Homogeneous chemical reaction (gas absorption by chemical solvent, Ex 5, convection only due to diffusion)

   ← *Penetration Model*

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1D Steady Diffusion

1D Steady Diffusion

1D Steady Diffusion, Problems Summary

✓ 1. Unimolecular mass transfer (evaporating tank, Ex 1; evaporating droplet, Ex 2)
   • Subcase: stagnant B, dilute A, $\underline{v}^* \approx 0$, $(\underline{N}_A \approx \underline{J}_A^*)$

   ← Film Model

✓ 2. Heterogeneous chemical reaction (catalytic converter, Ex 3, convection only due to diffusion)

✓ 3. Equimolar counter diffusion (distillation, $\underline{v}^* = 0$, $(\underline{N}_A = \underline{J}_A^*)$ Ex 4)

✓ 4. Homogeneous chemical reaction (gas absorption by chemical solvent, Ex 5, convection only due to diffusion)

   ← Penetration Model

Aside:

The ***film model*** and the ***penetration model*** will both appear again.

They are used as framings for ***lumped-parameter mass transfer models*** in complex unit operations. They differ in how they predict the mass transfer coefficient (*linear-driving-force model*) varies with diffusion coefficient.

Film: $k_c \propto D_{AB}$

Penetration: $k_c \propto D_{AB}^{\frac{1}{2}}$

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