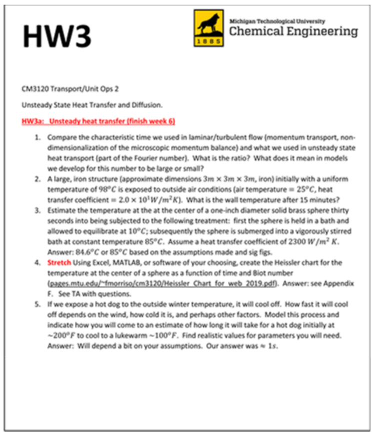
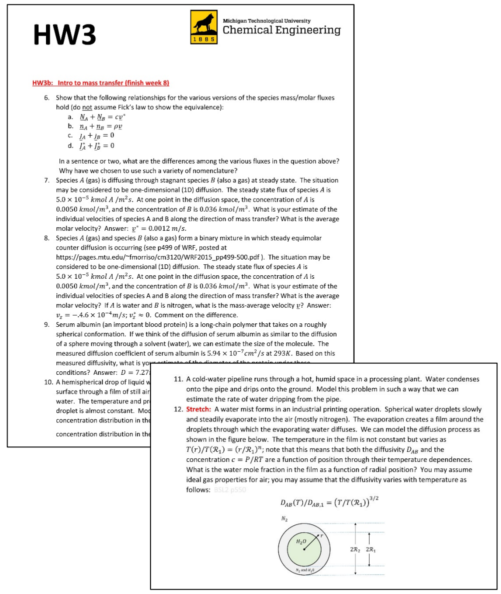
It's week 7. Next week is Week 8.
Exam 3: Week 9 (after break)

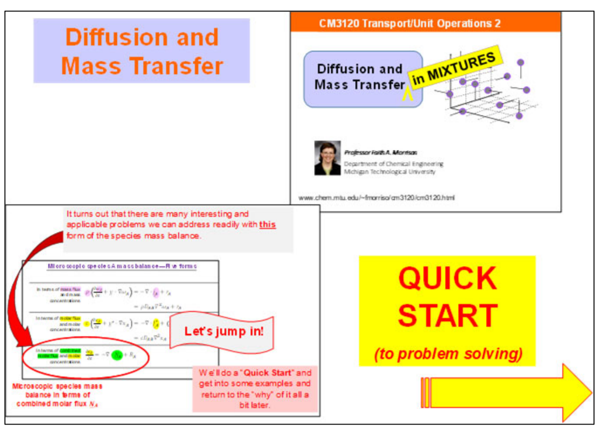
Homework 3A:
Finish Week 6




Homework 3B:
Finish Week 8






QUICK START

*(to problem solving)*

**Continuing…**

## Film model of mass transfer

QUICK START

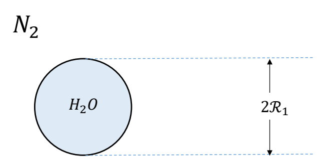
**Last time**, we did this second problem:

The primary goal is **to grow our ability to troubleshoot engineering problems.**

**EXAMPLE 2**

Let's do another problem

**Example 2**: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). What is the rate of evaporation and how does the water concentration vary in the gas?




Ver 1

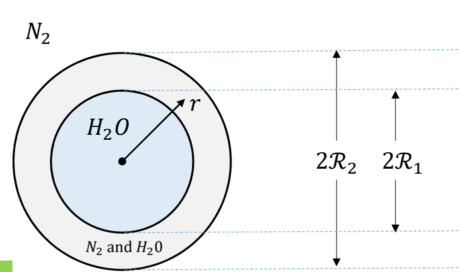
BSL2, p550

 3

## Film model of mass transfer

QUICK START

**Example 2**: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.




We *invented* the "film model"

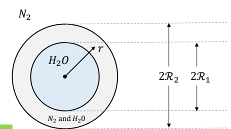
Ver 2

BSL2, p550

 4

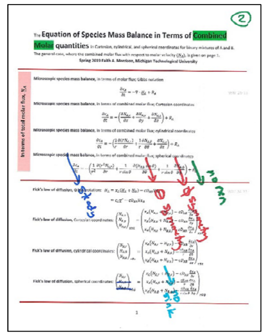
## Film model of mass transfer

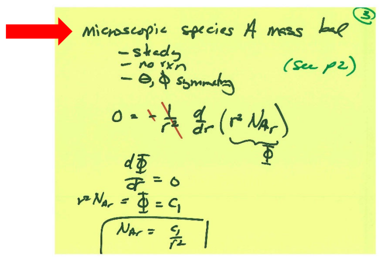
**Example 2**: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.

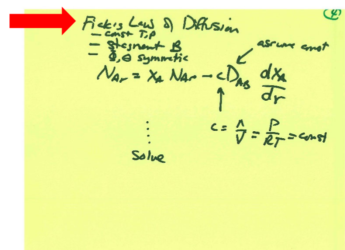



The Film Model of mass transfer

Ver 2






BSL2, p550

 5

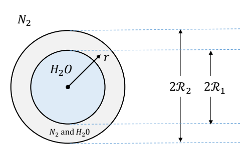
## Film model of mass transfer

QUICK START

Ver 2

*Assumptions*:
- Uniform film surrounds droplet
- Ideal gas
- Constant temperature and pressure

**Example 2**: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.




Ver 2

**Solution:**

$x_A(r)$

$$\frac{1 - x_A}{1 - x_{A1}} = \left(\frac{1 - x_{A2}}{1 - x_{A1}}\right)^{\left(\frac{\frac{1}{\mathcal{R}_1} - \frac{1}{r}}{\frac{1}{\mathcal{R}_1} - \frac{1}{\mathcal{R}_2}}\right)}$$

*Open: How would we "answer the question" in this problem?*

BSL2, p550

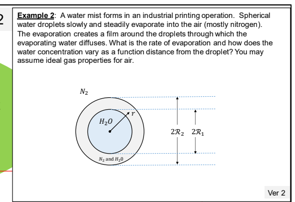
 6

QUICK START

We can now explore these assumptions, and modify, if needed, for more complex problems.

Ver 2

Assumptions:
- Uniform film surrounds droplet
- Ideal gas
- Constant temperature and pressure



**Solution:**

$x_A(r)$

$$\frac{1-x_A}{1-x_{A1}} = \left(\frac{1-x_{A2}}{1-x_{A1}}\right)^{\left(\frac{\frac{1}{\mathcal{R}_1}-\frac{1}{r}}{\frac{1}{\mathcal{R}_1}-\frac{1}{\mathcal{R}_2}}\right)}$$

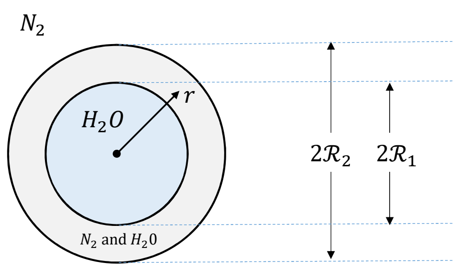
7



## Film model of mass transfer

QUICK START

**Example 2**: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air.




*Assumptions*:
- Uniform film
- Ideal gas
- Constant pressure
- Constant temperature

**Let's Interrogate the problem.**

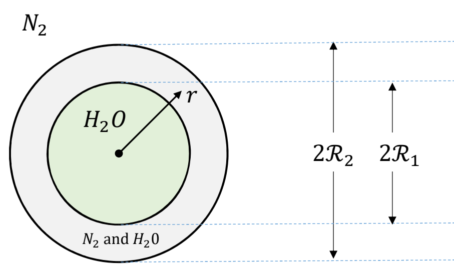
How good are these assumptions?

BSL2, p550

8

Film model of mass transfer (more complex) QUICK START

**Example 2**: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. We can model the diffusion process as shown in the figure. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet?




Note: *not* isothermal

$\Delta\hat{H}_{vap} \neq 0$

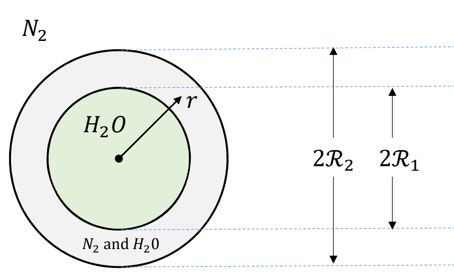
Ver 3

BSL2, p550

 9

Film model of mass transfer (more complex) QUICK START

**Example 2**: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. We can model the diffusion process as shown in the figure. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet?




Note: *not* isothermal

$\Delta\hat{H}_{vap} \neq 0$

*What does changing temperature impact?*

*How do we modify the model?*

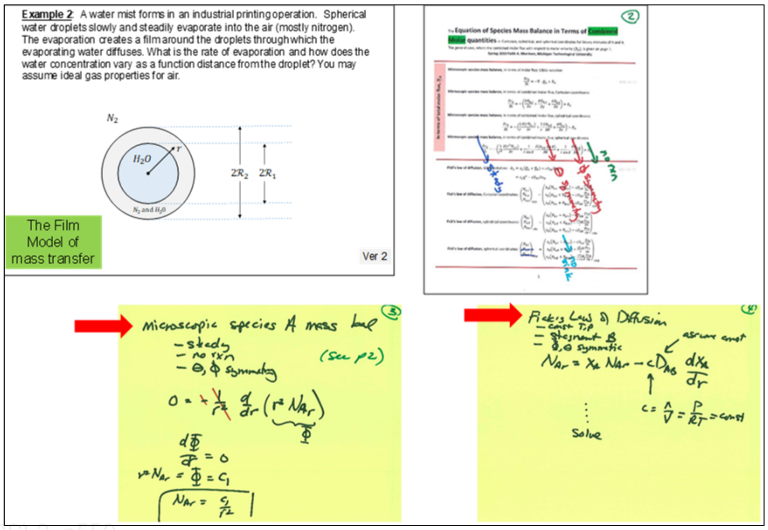
Ver 3

BSL2, p550

 10

## Film model of mass transfer (more complex)

Where did we assume "isothermal"?




BSL2, p550

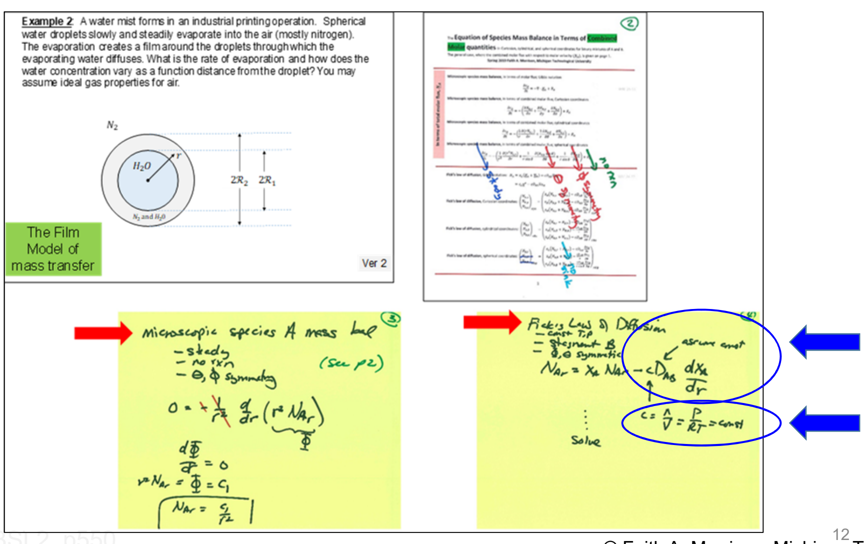
11



## Film model of mass transfer (more complex)

Where did we assume "isothermal"?

When we integrated to obtain $x_A(r)$.




BSL2, p550

12

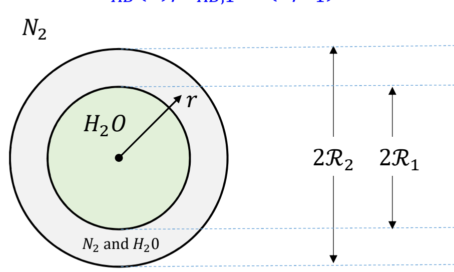
## Film model of mass transfer (more complex)

QUICK START

**Example 2**: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. We can model the diffusion process as shown in the figure. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$. What is the rate of evaporation and how does the water concentration vary as a function distance from the droplet? You may assume ideal gas properties for air; you may assume that the diffusivity varies with temperature as follows:

$$D_{AB}(T)/D_{AB,1} = (T/T_1)^{3/2}$$

Note: *not* isothermal




HW3, problem 12 **(stretch)**

Ver 4

BSL2, p550





## Film model of mass transfer (more complex)

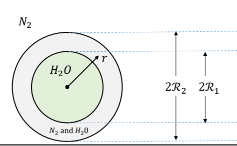
Ver 4

QUICK START

**Example 2**: A water mist forms in an industrial printing operation. Spherical water droplets slowly and steadily evaporate into the air (mostly nitrogen). The evaporation creates a film around the droplets through which the evaporating water diffuses. We can model the diffusion process as shown in the figure. The temperature in the film is not constant but varies as $T(r)/T(\mathcal{R}_1) = (r/\mathcal{R}_1)^n$. What is the water mole fraction in the film as a function of radial position? You may assume ideal gas properties for air; you may assume that the diffusivity varies with temperature as follows:

$$D_{AB}(T)/D_{AB,1} = (T/T_1)^{3/2}$$

Note: *not* isothermal




HW3, problem 12 **(stretch)**

*Assumptions*:

- Uniform film surrounds droplet
- Ideal gas
- Temperature follows power law
- Diffusivity follows power law
- Pressure is constant

**Solution:**

$x_A(r)$

$$\frac{1-x_A}{1-x_{A1}} = \left(\frac{1-x_{A2}}{1-x_{A1}}\right)^{\left(\frac{\frac{1}{\mathcal{R}_1^{1+n/2}}-\frac{1}{r^{1+n/2}}}{\frac{1}{\mathcal{R}_1^{1+n/2}}-\frac{1}{\mathcal{R}_2^{1+n/2}}}\right)}$$

BSL2, p550

The primary goal is **to grow our ability to troubleshoot engineering problems.**

QUICK START

## Let's do another problem, more complex

**EXAMPLE 3**

**Example 3:** Heterogeneous catalysis

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

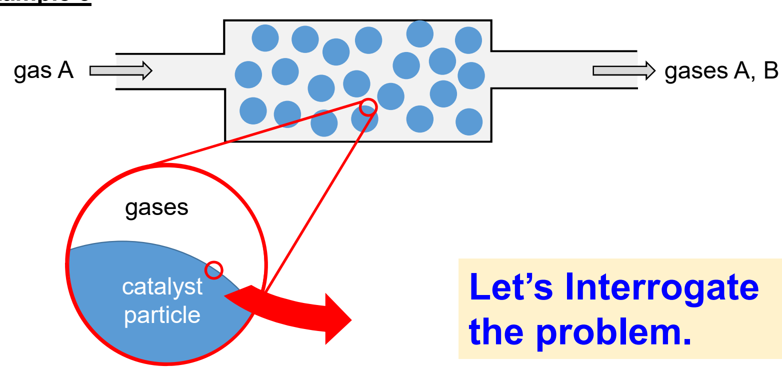
BSL2, p550

 15

Film model of mass transfer (more complex)

QUICK START

**Example 3**




**Let's Interrogate the problem.**

**Example 3:** Heterogeneous catalysis
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?

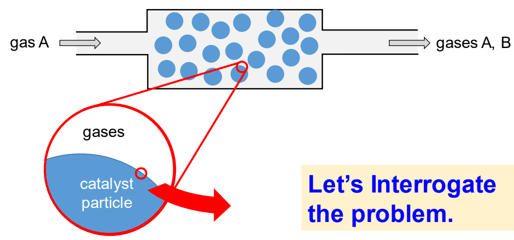
BSL2, p552

 16

QUICK START

# Let's Interrogate the problem.

**Example 3**




**Example 3**: Heterogeneous catalysis
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?

*What is the geometry? What does it affect?*

*How does diffusion affect how fast the chemical transformation takes?*

*How would diffusion take place (look for sources, sinks)*

*What is the governing physics?*

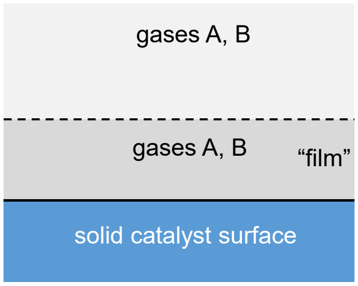
BSL2, p552

 17

## Film model of mass transfer (more complex)

QUICK START

**Example 3**: 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 $x_A(z)$ and the flux of product $B$ away from the surface.



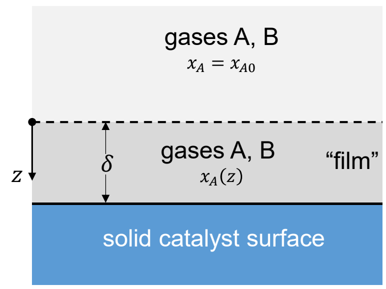

BSL2, p552

 18

## Film model of mass transfer (more complex)

QUICK START

**Example 3:** 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 $x_A(z)$ and the flux of product $B$ away from the surface.

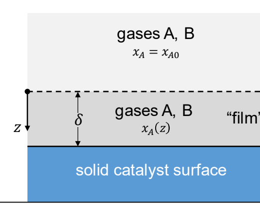



- Deploy the "film model"
- It has become *a way of thinking about* diffusion in some circumstances




QUICK START

**Example 3:** 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 ($x_A(z)$) and the flux of product $B$ away from the surface.




**SOLVE**

BSL2, p550

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

The general case, where the combined molar flux with respect to molar velocity ($\underline{N}_A$), is given on page 1.

**Spring 2019 Faith A. Morrison, Michigan Technological University**

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

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

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

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

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

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

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

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

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

21



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

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

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

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

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

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

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

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

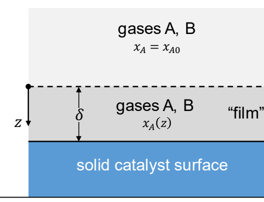
$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r\sin\theta}\frac{\partial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

22

QUICK START

# SOLUTION:

**Example 3:** 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 ($x_A(z)$) and the flux of product $B$ away from the surface.




## See hand slides for start; solution assigned in HW4

BSL2, p550

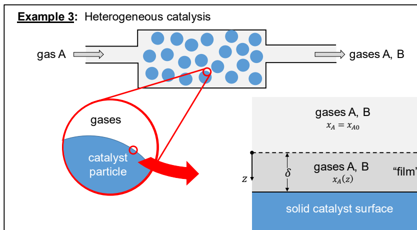
23



Film model of mass transfer (more complex)

*Assumptions*:
- Fast, irreversible reaction at surface
- Diffusion through film at surface limits rate of reaction
- Steady state
- Constant T, P

**Example 3:** 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 ($x_A(z)$) and the flux of product $B$ away from the surface.

## Solution:

$x_A(z)$

$$\left(1-\frac{1}{2}x_A\right) = \left(1-\frac{1}{2}x_{A0}\right)^{(1-z/\delta)}$$

*Open: How would we "answer the question" in this problem?*

BSL2, p550

24

Introduction to Diffusion and Mass Transfer in Mixtures QUICK START

## Recurring Modeling Assumptions in Diffusion

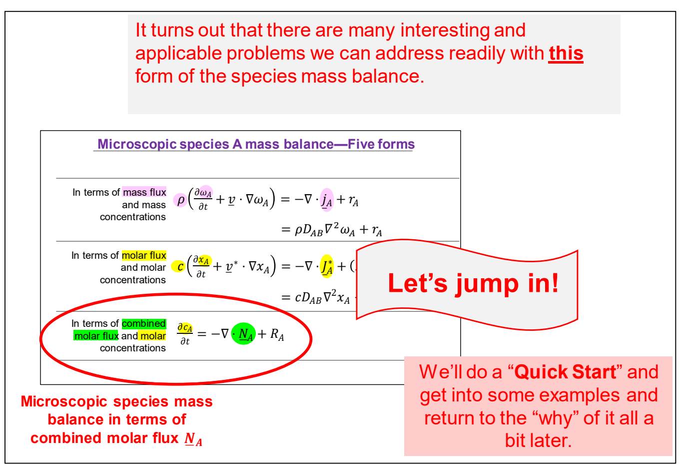
- Near a liquid-gas interface, the region in the gas near the liquid is a film where slow diffusion takes place
- The vapor near the liquid-gas interface is often saturated (Raoult's law, $x_A = p_A^*/p$)
- If component $A$ has no sink, $\underline{N}_A = 0$.
- If $A$ diffuses through stagnant $B$, $\underline{N}_B = 0$.
- If, for example, two moles of $A$ diffuse to a surface at which a rapid, irreversible reaction coverts it to one mole of $B$, then at steady state $-0.5\underline{N}_A = \underline{N}_B$.
- Because diffusion is slow, we can make a quasi-steady-state assumption
- Homogeneous reactions appear in the mass balance; heterogeneous reactions appear in the boundary conditions
- If a binary mixture of $A$ and $B$ are undergoing steady equimolar counter diffusion, $\underline{N}_A = -\underline{N}_B$. (coming)
-
-

25



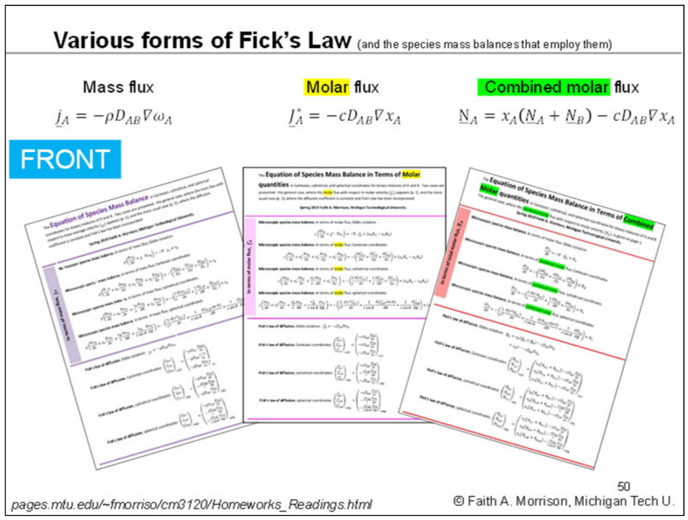
## We have been performing a "Quick Start,"

### And have found the **combined molar flux** formulation useful.




26

There are times it is not useful. We need to go back and discuss *how/why/when* this all works.

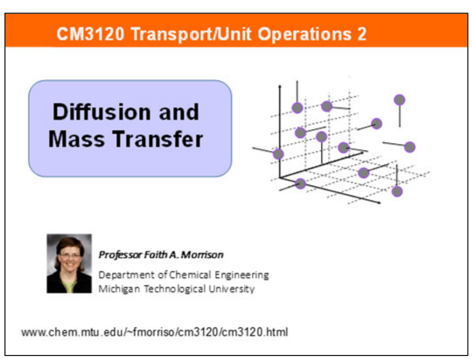



27



# Now, Cycling Back:

## Diffusion and Mass Transfer




28