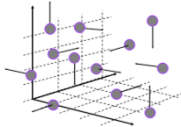



Diffusion/Mass Transfer Recap and Planning

CM3120 Transport/Unit Operations 2

Diffusion and Mass Transfer





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

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

Where are we?

Time for a recap.

➔

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Diffusion/Mass Transfer Recap and Planning

Recap:
Diffusion/Mass Transfer (so far, and beyond)

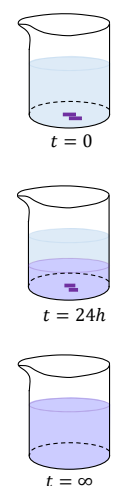
Mixtures

Diffusion:

- Brownian motion (random molecular motion),
- Fick's law of diffusion, D_{AB}
- slow,
- operates over short distances

Mass Transfer:

- Includes all mechanisms (e.g. diffusion, convection, thermodynamics-driven),
- Linear-driving-force model,
- slow,
- also acts over short distances but convection extends it a bit



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Diffusion/Mass Transfer Recap and Planning

Recap:
Diffusion/Mass Transfer (so far, and beyond)

Mixtures

Diffusion:

- Brownian motion (random molecular motion),
- Fick's law of diffusion, D_{AB}
- slow,
- operates over short distances

Mass Transfer:

- Includes all mechanisms convection, thermodynamic
- Linear-driving-force model, Haven't actually talked about this yet
- slow,
- also acts over short distances but convection extends it a bit

$t = 0$

$t = 24h$

$t = \infty$

3

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Diffusion/Mass Transfer Recap and Planning

Recap:
Diffusion/Mass Transfer (so far, and beyond)

Modeling:

Microscopic species A mass balance
(continuum modeling tricky with mixtures; also issues of units, (mass versus moles) and reference coordinates)

- Four fluxes $\underline{N}_A, \underline{J}_A^*, \underline{n}_A, \underline{j}_A$
- Three summary sheets using $\underline{N}_A, \underline{J}_A^*, \underline{j}_A$

Fick's law (diffusion)

- Diffusion coefficient D_{AB}
- Four forms using $\underline{N}_A, \underline{J}_A^*, \underline{n}_A, \underline{j}_A$

Linear-driving-force model (mass transfer; analogous to Newton's law of cooling)—
mass transfer coefficient $k_{various\ designations}$

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

Mass flux $\underline{J}_A = -\rho D_{AB} \nabla x_A$	Molar flux $\underline{J}_A^* = -c D_{AB} \nabla x_A$	Continuum flux $\underline{N}_A = x_A (\underline{E}_A + \underline{D}_A) - c D_{AB} \nabla x_A$
----------------------------------------------------------	-----------------------------------------------------------------	------------------------------------------------------------------------------------------------------------

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Diffusion/Mass Transfer Recap and Planning

Recap:
Diffusion/Mass Transfer (so far, and beyond)

Modeling:

Microscopic species A mass balance
(continuum modeling tricky with mixtures; also issues of units, (mass versus moles) and reference coordinates)

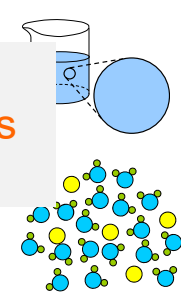
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Fick's law (diffusion)

- Diffusion coefficient D_{AB}
- Four forms using $\underline{N}_A, \underline{J}_A^*, \underline{n}_A, \underline{j}_A$

Linear-driving-force model (mass transfer; analogous to Newton's law of cooling)—mass transfer coefficient $k_{various\ designations}$


Have not touched this yet



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

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



Diffusion/Mass Transfer Recap and Planning

Recap:
Diffusion/Mass Transfer (so far, and beyond)

Modeling:

Microscopic species A mass balance
(continuum modeling tricky with mixtures; also issues of units, (mass versus moles) and reference coordinates)

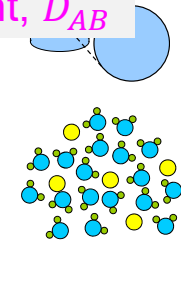
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- Three summary sheets using $\underline{N}_A, \underline{J}_A^*, \underline{j}_A$

Fick's law (diffusion)

- Diffusion coefficient D_{AB}
- Four forms using $\underline{N}_A, \underline{J}_A^*, \underline{n}_A, \underline{j}_A$

Linear-driving-force model (mass transfer; analogous to Newton's law of cooling)—mass transfer coefficient $k_{various\ designations}$

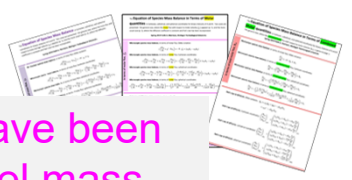
Up to now, we have been learning to model mass transfer using Fick's law and the diffusion coefficient, D_{AB}



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

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



Diffusion/Mass Transfer Recap and Planning

Recap: Diffusion/Mass Transfer (so far, and beyond)

We did a Quick Start:

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

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

Learning to use the microscopic species A balance

Various forms of Fick's Law (and the appropriate balance that applies them!)

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

and later, **Cycled Back:**

Example

Water (at 20°C, 1.0 atm) slowly and steadily evaporates into nitrogen (at 20°C, 1.0 atm) from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. The geometry is as shown in the figure. What is water mole fraction as a function of vertical position? You may assume ideal gas properties. What is the rate of water evaporation?

Example

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. What is the water mole fraction in the film as a function of radial position? You may assume ideal gas properties for air.

Example

Heterogeneous catalysis

An irreversible, instantaneous chemical reaction (2A → 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 (μ, x_A).

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Diffusion/Mass Transfer Recap and Planning

Recap: Diffusion/Mass Transfer (so far, and beyond)

Cycle Back:

- Origin of Fick's law—Brownian motion
- Reasons for various fluxes—diffusion and bulk motion challenging to separate experimentally
- When to use various fluxes—depends on what we know about the problem

Simple One-dimensional, Species Mass Diffusion

At steady state, $\omega_A(y, t) = -\frac{cA_0}{D}y + \omega_{A,0}$

flux = $\rho D_{AB} \left(\frac{0 - \omega_{A,0}}{y_2 - y_1} \right)$

$\underline{J}_{A,y} = -\rho D_{AB} \frac{d\omega_A}{dy}$

Fick's law of diffusion (in terms of mass flux)

D_{AB} = Diffusion coefficient of A through B
 $\underline{J}_{A,y}$ = mass flux of A through B

Various forms of Fick's Law

Summary:

Possible fluxes so far:

$\underline{J}_A^* = (v_A - v^*)c_A$ = molar flux relative to molar average velocity v^*
 $\underline{J}_A = (v_A - v^*)\rho c_A$ = mass flux relative to mass average velocity v^*

Combined fluxes are also in use:

\underline{N}_A = combined molar flux relative to stationary coordinates
 \underline{B}_A = combined mass flux relative to stationary coordinates

Mass: $\underline{J}_A = \rho v_A(v_A - v^*) = \rho v_A v_A - \rho v_A v^* = \rho v_A v_A - \rho v_A v^*$
 $\underline{B}_A = \underline{J}_A + \rho v_A v^* = \rho v_A v_A$

Moles: $\underline{J}_A^* = c_A(v_A - v^*) = c_A v_A - c_A v^*$
 $\underline{N}_A = \underline{J}_A^* + c_A v^* = c_A v_A$

All our previous flux expressions (momentum and energy) have been with respect to stationary coordinates. In diffusion, this points to the combined fluxes.

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Let's put this to use

Microscopic species A mass balance—Stoichiometric form

In terms of mass flux and mass average velocity:

$$\rho \left(\frac{\partial \omega_A}{\partial t} + v^* \omega_A \right) = -\nabla \cdot \underline{B}_A + R_A$$

$$= -\rho v_A \nabla \omega_A + R_A$$

In terms of molar flux and molar average velocity:

$$\rho c_A \left(\frac{\partial x_A}{\partial t} + v^* x_A \right) = -\nabla \cdot \underline{N}_A + R_A$$

$$= -c_A v_A \nabla x_A + R_A$$

Diffusion/Mass Transfer Recap and Planning

Recap:
Diffusion/Mass Transfer (so far, and beyond)

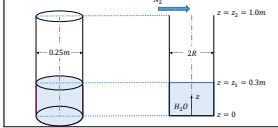
Problems Solved
(1D), Steady:

- Unimolecular mass transfer
- Heterogeneous chemical reaction
- Equimolar counter diffusion
- Homogeneous chemical reaction

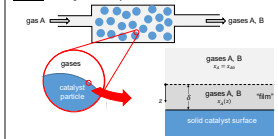
Applied to Unit Operations:

- Evaporation (tank)
- Catalytic reactors
- Distillation
- Absorption

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

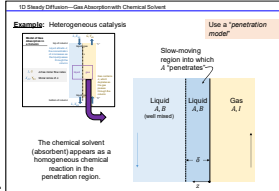


b. **Example: Heterogeneous catalysis**



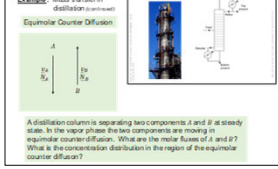
An irreversible, instantaneous chemical reaction ($2A \rightarrow B$) takes place at a catalyst surface, as shown. The reaction is "diffusion-limited," however, because the rate of completion of the reaction is determined by the rate of diffusion through the "film" near the catalyst surface. Calculate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

d.



The chemical solvent (absorbent) appears as a homogeneous chemical reaction in the penetration region. Use a "penetration model".

c.



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 diffusion?

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Diffusion/Mass Transfer Planning

... and beyond

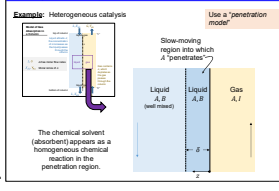
For all these problems we used the N_A approach:

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

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

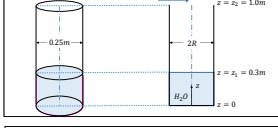
Why?

d.

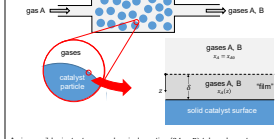


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a. **Example:** Water (40°C, 1.0 atm) slowly and steadily evaporates into nitrogen (40°C, 1.0 atm) from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water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

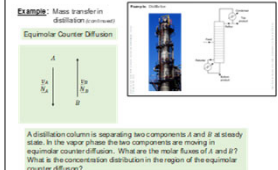


b. **Example: Heterogeneous catalysis**



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 ($x_A(x,z)$).

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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 diffusion?

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Diffusion/Mass Transfer Planning

For all these problems we used the \underline{N}_A approach:

Why?

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

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

Because we were able to say something about the convection term.

In these problems, convection was caused by diffusion only.

Diffusion/Mass Transfer Planning

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Diffusion/Mass Transfer Planning

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Diffusion/Mass Transfer Planning

Microscopic species A mass balance

convection

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

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

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

combined convection and diffusion

Diffusion/Mass Transfer Planning

For all these problems we used the \underline{N}_A approach:

Why?

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

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Diffusion/Mass Transfer Planning

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Diffusion scenarios are **MUCH more complicated** when the convection includes additional **bulk** motion caused by: pressure variation, gravity, etc.


Yet, this includes most situations. ?

Diffusion/Mass Transfer Planning

Recap:
Diffusion/Mass Transfer (so far, and beyond)

CM3120 Transport/Unit Operations 2

Diffusion and Mass Transfer *in MIXTURES*




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

Our topic is **Diffusion and Mass Transfer**

We have covered **DIFFUSION**, which includes modeling species mass transfer with **Fick's law of Diffusion** and the diffusion coefficient D_{AB} .

This is suitable, and convenient for cases when there is **little bulk convection accompanying the diffusion**.


When there is **appreciable bulk convection** accompanying the diffusion, we need another approach.



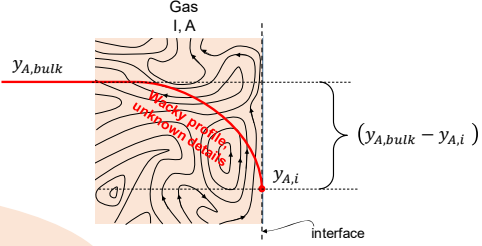
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Linear Driving Force Model for Mass Transfer

CM3110
 Transport II
 Part II: Diffusion and Mass Transfer




Michigan Tech



Linear Driving Force Model for Mass Transfer

$$|N_A| = k_y |y_{A,bulk} - y_{A,i}|$$



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

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Bulk convection present- Linear-driving-force model

Consider a less idealized situation:

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

e.g. gas absorption

Both fluids are **in motion**

Gas I, A

Liquid B

$y_{A,bulk}$

$x_{A,bulk}$

interface

Bulk flow is present.

\underline{v} in both phases is complicated, not zero

?

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WRF, Ch29 p 596

Bulk convection present- Linear-driving-force model

Consider a less idealized situation:

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

e.g. gas absorption

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Gas I, A

Liquid B

$y_{A,bulk}$

$x_{A,bulk}$

interface

Bulk flow is present.

\underline{v} in both phases is complicated, not zero

?

What can we do?

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Bulk convection present- Linear-driving-force model

Remember Newton's law of cooling?

CM3110

What about this case?

Example 2: Heat flux in a rectangular solid – Fluid BC

What is the steady state temperature profile in a wide rectangular slab if one side is exposed to fluid at T_b ?

$T_b \neq T_{wall}$

What is the flux at the wall?

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Bulk convection present- Linear-driving-force model

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CM3110

What about this case?

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Bulk convection present- Linear-driving-force model

Remember Newton's law of cooling?

CM3110
 An Important Boundary Condition in Heat Transfer: **Newton's Law of Cooling**

We want an easier way to handle this common situation.

The fluid is in motion

We'll solve an idealized case, nondimensionalize, take data and correlate!

What is the flux at the wall?

$T_b \neq T_{wall}$
 $v(x, y, z) \neq 0$

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Bulk convection present- Linear-driving-force model

Remember Newton's law of cooling?

= linear-driving-force model

The flux at the wall is given by the empirical expression known as **Newton's Law of Cooling**

Newton's law of cooling assumes the heat flux is **proportional to the driving force, ΔT**

$\Delta T = T_{bulk} - T_{wall}$

This is a **linear-driving-force model** for heat transfer at an interface

This expression serves as the definition of the **heat transfer coefficient**.

$$\left| \frac{q_x}{A} \right| = h |T_{bulk} - T_{wall}|$$

h depends on:

- geometry
- fluid velocity field
- fluid properties
- temperature difference

For now, we'll "hand" you **h**; later, you'll get it from **literature correlations**.

The flux at the wall is given by the empirical expression known as **Newton's Law of Cooling**

$T_b \neq T_{wall}$
 $v(x, y, z) \neq 0$

What is the flux at the wall?

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Bulk convection present- Linear-driving-force model

Remember *Newton's law of cooling*?

With this model, we lump all the complexity in the bulk fluid phase into h and use data correlations (experimental data) to get final numbers.

The temperature difference at the fluid-wall interface is caused by complex phenomena that are lumped together into the heat transfer coefficient, h

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Bulk convection present- Linear-driving-force model

Summary – Heat transfer coefficient, h

- Newton's law of cooling is a **linear-driving-force model** for heat transfer at a boundary
- The "real" physics at the boundary is governed by the microscopic energy balance, but it's too hard to solve
- We non-dimensionalize the governing equations for the problem of interest (e.g. forced convection, natural convection, boiling, condensation)
- This identifies the appropriate **dimensionless numbers**
- We take data and **correlate** using the dimensionless numbers
- h represents a "resistance" to heat transfer at the boundary
- Multiple resistances may be combined to yield an "overall" **heat transfer coefficient U** that may be used in equipment design.

The flux at the wall is given by the empirical expression known as **Newton's Law of Cooling**

This expression serves as the definition of the heat transfer coefficient.

$$\frac{q_x}{A} = h|T_{bulk} - T_{wall}|$$

h depends on:

- geometry
- fluid velocity field
- fluid properties
- temperature difference

For now, we'll "hand" you h ; later, you'll get it from literature correlations.

We can do the same with mass transfer coefficient:

- **linear-driving force model**
- **dimensionless numbers**
- **correlations**
- **overall mass-transfer coefficient**

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Bulk convection present- Linear-driving-force model

Inspiration:

We now do the same with mass transfer coefficient:

- linear-driving force model
- dimensionless numbers
- correlations
- overall mass-transfer coefficient

This is a **linear-driving-force model** for mass transfer at an interface

$$|N_A| = k_y |y_{A,bulk} - y_{A,i}|$$

(set signs by the situation)

This equation serves as the defining equation for mass transfer coefficient (based on gas mole fraction; **there will be others with other units**) (sorry about that)

The flux at the wall is given by the empirical expression known as **Newton's Law of Cooling**

$\frac{q_x}{A} = h |T_{bulk} - T_{wall}|$

Summary – Heat transfer coefficient, h

- Newton's law of cooling is a **linear-driving-force model** for heat transfer at a boundary
- The "real" physics at the boundary is governed by the microscopic energy balance, but it's too hard to solve
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- Multiple resistances may be combined to yield an "overall" heat transfer coefficient U that may be used in equipment design.

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Bulk convection present- Linear-driving-force model

For mass transfer:

Linear-driving-force model: the flux of A from the bulk in the gas is proportional to the difference between the bulk composition and the composition at the interface.

$$N_A = k_y (y_{A,bulk} - y_{A,i})$$

This is the defining equation for the mass-transfer coefficient, k_y

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WRF, Ch29 p 596

Bulk convection present- Linear-driving-force model

Linear-driving-force model: the flux of A from the bulk in the gas is proportional to the difference between the bulk composition and the composition at the interface.

The defining equations for the mass-transfer coefficients:

$$N_A = k_y (y_{A,bulk} - y_{A,i}) \quad k_y [=] \frac{\text{moles } A}{\text{cm}^2 \text{ s}}$$

$$N_A = k_c (c_{A,bulk} - c_{A,i}) \quad k_c [=] \frac{\text{cm}}{\text{s}}$$

(gases) $N_A = \frac{k_c}{RT} (p_{A,bulk} - p_{A,i})$ (sometimes called "diffusion velocity")

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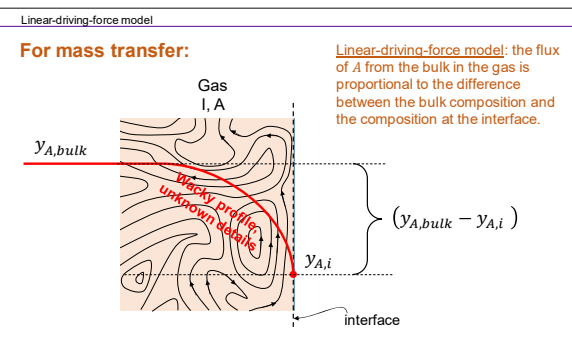
Bulk convection present- Linear-driving-force model

With this method, we do not model **the details** of the diffusion and convection in the gas.

Instead, we propose that **the net effect** is that flux is proportional to the **driving force** Δy_A (or Δc_A or Δp_A)

Linear-driving-force model

For mass transfer:




Linear-driving-force model: the flux of A from the bulk in the gas is proportional to the difference between the bulk composition and the composition at the interface.

This is the defining equation for the mass transfer coefficient, k_y

$$N_A = k_y (y_{A,bulk} - y_{A,i})$$

Let's take it out for a spin with some familiar solutions.



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Bulk convection present- Linear-driving-force model

Example: The film model of 1D steady diffusion yields a composition distribution and an expression for the flux. What is the mass-transfer coefficient in the film model?

(we use x for liquid and y for gas mole fractions)

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Bulk convection present- Linear-driving-force model

Example: The film model of 1D steady diffusion yields a composition distribution and an expression for the flux. What is the mass-transfer coefficient in the film model?

You try.

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Bulk convection present- Linear-driving-force model

Example: The film model of 1D steady diffusion yields a composition distribution and an expression for the flux. What is the mass-transfer coefficient in the film model?

Solution:

$$k_y = \frac{cD_{AB}}{\delta} \left[\frac{\ln\left(\frac{y_{B2}}{y_{B1}}\right)}{(y_{B2} - y_{B1})} \right]$$

$$y_{B,lm} \equiv \frac{(y_{B2} - y_{B1})}{\ln\left(\frac{y_{B2}}{y_{B1}}\right)}$$

$$k_y = \frac{cD_{AB}}{\delta (y_{B,lm})}$$

Film model prediction for mass-transfer coefficient

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Bulk convection present- Linear-driving-force model

Example: The film model of 1D steady diffusion yields a composition distribution and an expression for the flux. What is the mass-transfer coefficient in the film model?

Solution:

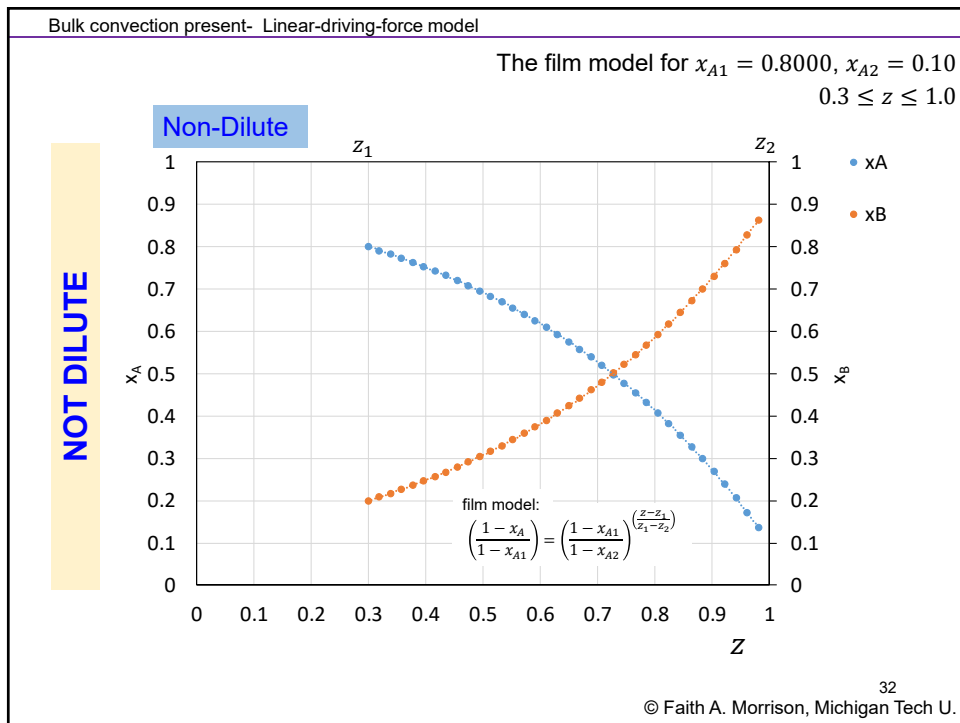
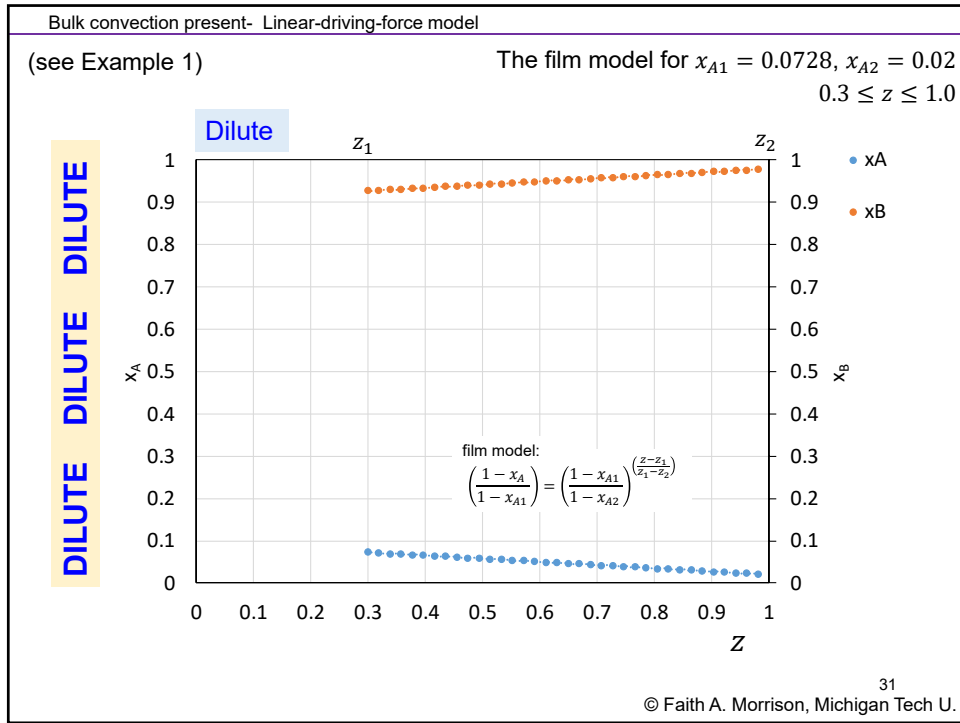
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Film model prediction for mass-transfer coefficient

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Bulk convection present- Linear-driving-force model

Mass-transfer coefficient for film model

We used mole fraction units:

$$N_A = k_y (y_{A,bulk} - y_{A,i})$$

For gases we often use concentration units and assume ideal gas:

$$N_A = k_c (c_{A,bulk} - c_{A,i})$$

$$c = \frac{n}{V} = \frac{P}{RT}$$

...

$$k_c = \frac{PD_{AB}}{\delta (P_{B,lm})}$$

Film model prediction for mass transfer coefficient

WRF eqn 26-9

film model

$$k_c \propto D_{AB}$$

33

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Bulk convection present- Linear-driving-force model

Example: The penetration model of 1D steady diffusion yields a composition distribution and an expression for the flux. What is the mass-transfer coefficient in the penetration model?

(we use x for liquid and y for gas mole fractions)

Gas
I, A

flux of A
→

Liquid
B

34

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Bulk convection present- Linear-driving-force model

Example: The penetration model of 1D steady diffusion yields a composition distribution and an expression for the flux. What is the mass-transfer coefficient in the penetration model?

You try.

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Bulk convection present- Linear-driving-force model

Example: The penetration model of 1D steady diffusion yields a composition distribution and an expression for the flux. What is the mass-transfer coefficient in the penetration model?

Solution:

$$N_A = \frac{D_{AB} c_{A0}}{\delta} \left(\frac{\delta \sqrt{k_1/D_{AB}}}{\tanh(\delta \sqrt{k_1/D_{AB}})} \right)$$

$$= k_c (c_{A0} - 0)$$

$$k_c = \frac{D_{AB}}{\delta} \left(\frac{\delta \sqrt{k_1/D_{AB}}}{\tanh(\delta \sqrt{k_1/D_{AB}})} \right)$$

Penetration model prediction for mass transfer coefficient

As k_1 becomes large,

$k_c = \sqrt{k_1 D_{AB}}$

Penetration model prediction for mass transfer coefficient, large k_1

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

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Mass Transport "Laws" ——— **Summary** ———

We now have 2 Mass Transport "laws"

Fick's Law of Diffusion $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$ Transport coefficient

Use: Combine with microscopic species *A* mass balance
 Predicts flux \underline{N}_A and composition distributions, e.g. $x_A(x, y, z, t)$
 1D Steady models can be solved
 1D Unsteady models can be solved (if good at math)
 2D steady and unsteady models can be solved by Comsol
 Since we predict \underline{N}_A , we can also predict a mass xfer coeff k_y or k_c
 Diffusion coefficients are **material properties** (see tables)

Linear-Driving-Force Model $|N_A| = k_y|y_{A,bulk} - y_{A,i}|$

Use: Combine with macroscopic species *A* mass balance
 Predicts flux \underline{N}_A , but not composition distributions
 May be used as a boundary condition in microscopic balances
 Mass-transfer-coefficients are **not material properties**
 Rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations)
 Facilitate combining resistances into overall mass xfer coeffs, K_L, K_G

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Mass Transport "Laws"

We now have 2 Mass Transport "laws"

Remaining Topics
 to round out our understanding of mass transport

Fick's Law of Diffusion $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

Use: ✓ Combine with microscopic species A mass balance
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Linear-Driving-Force Model $|N_A| = k_y|y_{A,bulk} - y_{A,i}|$

Use: Combine with macroscopic species A mass balance 3
 Predicts flux \underline{N}_A , but not composition distributions
 May be used as a boundary condition in microscopic balances
 Mass-transfer-coefficients are **not material properties**
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 Facilitate combining resistances into overall mass xfer coeffs, K_L, K_G 5

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Mass Transport "Laws"

We now have 2 Mass Transport "laws"

Remaining Topics to round out our understanding of mass transport:

Fick's law of diffusion

D_{AB} {

- Since we predict \underline{N}_A with Fick's law, we can also predict a mass transfer coefficients k_y or k_c
- 1D Unsteady models can be solved (if good at math)

Mass transfer coefficients

k_c {

- Combine with macroscopic species A mass balance
- Are not material properties; rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations)
- Facilitate combining resistances into overall mass transfer coefficients, K_L, K_G , to be used in modeling unit operations

Mass Transport "Laws"

We now have 2 Mass Transport "laws"

Transport coefficient

Fick's Law of Diffusion $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

Use: Combine with microscopic species A mass balance
 Predicts flux \underline{N}_A and composition distributions, e.g. $x_A(x, y, z, t)$
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Mass Transport "Laws"

We now have 2 Mass Transport "laws"

Remaining Topics to round out our understanding of mass transport:

Fick's law of diffusion

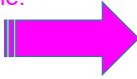
D_{AB} {

1. Since we predict N_A with Fick's law, we can also predict a mass transfer coefficient k_y or k_c
2. 1D Unsteady models can be solved (if good at math)

Mass transfer coefficients

k_c {

3. Combine with macroscopic species A mass balance
4. Are not material properties; rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations)
5. Facilitate combining resistances into overall mass transfer coefficients, K_L, K_G , to be used in modeling unit operations

We'll take them one at a time. 

Mass Transport "Laws"

We now have 2 Mass Transport "laws" Transport coefficient

Fick's Law of Diffusion $N_A = x_A(\dot{N}_A + \dot{N}_B) - cD_{AB}\nabla^2 x_A$

Use: Combine with microscopic species A mass balance
Predicts flux N_A and composition distributions, e.g. $x_A(x, y, z, t)$

1D Steady models can be solved

1D Unsteady models can be solved (if good at math) ②

2D steady and unsteady models can be solved by COMSOL

Since we predict N_A , we can also predict a mass xfer coeff k_y or k_c ①

Diffusion coefficients are **material** properties (see tables)


Linear-Driving-Force Model $|N_A| = k_y |y_{A, bulk} - y_{A, i}|$

Use: Combine with macroscopic species A mass balance
Predicts flux N_A , but **not** composition distributions
May be used as a boundary condition in microscopic balances
Mass-transfer-coefficients are **not material properties**
Rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations) ④

Facilitate combining resistances into overall mass xfer coeffs, K_L, K_G ⑤

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Predicting Mass Transfer Coefficients


 Michigan Tech

CM3110
Transport II
Part II: Diffusion and Mass Transfer

Predicting Mass-Transfer Coefficients
From solutions to the microscopic species A mass balance

①

Model	Basic Form	$f(D_{AB})$
Film theory	$k_c = \frac{D_{AB}}{\delta}$	$k_c \propto D_{AB}$
Falling liquid film	$k_c = \sqrt{\frac{4D_{AB}v_{\infty}}{\pi L}}$	$k_c \propto D_{AB}^{1/2}$
Penetration theory	$k_c = \sqrt{\frac{4D_{AB}}{\pi t_{exp}}}$	$k_c \propto D_{AB}^{1/2}$
Boundary-layer theory	$k_c = 0.664 \frac{D_{AB}}{L} \text{Re}_L^{1/2} \text{Sc}_L^{1/3}$	$k_c \propto D_{AB}^{2/3}$



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Department of Chemical Engineering
Michigan Technological University

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Mass Transport "Laws"

1 Since we predict N_A with Fick's law, we can also predict a mass transfer coefficients k_y or k_c with Fick's law

Mass Transport "Laws"

We now have 2 Mass Transport "laws"

Fick's Law of Diffusion $N_A = x_A(u_A + N_A) - cD_{AB} \frac{dx_A}{dy}$

Use: Combine with microscopic species A mass balance
 Predicts flux N_A and composition distributions, e.g. $x_A(x,y,z,t)$
 1D Steady models can be solved
 1D Unsteady models can be solved (if good at math)
 2D steady and unsteady models can be solved by COMSOL
 Since we predict N_A , we can also predict a mass xfer coeff k_y or k_c
 Diffusion coefficients are material properties (see tables)

Linear-Driving-Force Model $|N_A| = k_y(y_{A,s} - x_A)$

Use: Combine with macroscopic species A mass balance
 Predicts flux N_A , but not composition distributions
 May be used as a boundary condition in microscopic balances
 Mass transfer coefficients are **not** material properties
 Rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations)
 Facilitate combining resistances into overall mass xfer coeffs, K_y, K_c

$$k_c = \frac{PD_{AB}}{\delta(P_{B,lm})}$$

Film model prediction for mass transfer coefficient

film model

$$k_c \propto D_{AB}$$

As k_1 becomes large,

$$k_c = \sqrt{k_1 D_{AB}}$$

Penetration model prediction for mass transfer coefficient, large k_1

penetration model

$$k_c \propto D_{AB}^{1/2}$$

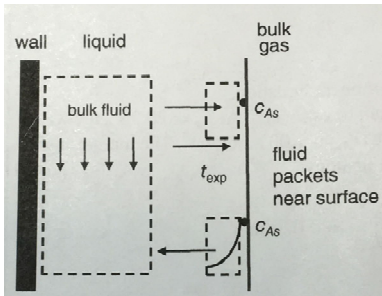
These predictions can be used to infer what physics is controlling mass transfer in a unit:

- diffusion through a stagnant film (film model, $k_c \propto D_{AB}$) or
- time of exposure for penetration ($k_c \propto D_{AB}^{1/2}$, penetration model).

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Mass Transport "Laws"

Another physical picture associated with penetration theory is "surface renewal" (Danckwerts)



- Turbulent flow
- Diffusing species only penetrates a short distance
- Due to chemical reaction or short time of contact, t_{exp}
- Model as unsteady state molecular transport
- Danckwerts: Bulk motion brings fresh liquid eddies from interior to the surface
- At the surface A is transferred as though B were stagnant and infinitely deep
- Works for falling film

$$k_c = \sqrt{\frac{4D_{AB}}{\pi t_{exp}}}$$

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WRF, Ch28 p 584

Mass Transport "Laws" **SUMMARY**

1 Since we predict N_A with Fick's law, we can also predict a mass transfer coefficients k_y or k_c with Fick's law and a model

Model	Basic Form	$f(D_{AB})$	Notes
Film theory	$k_c = \frac{D_{AB}}{\delta}$	$k_c \propto D_{AB}$	δ unknown
Falling liquid film	$k_c = \sqrt{\frac{4D_{AB}v_\infty}{\pi L}}$	$k_c \propto D_{AB}^{1/2}$	Solute does not penetrate very far into the liquid film
Penetration theory	$k_c = \sqrt{\frac{4D_{AB}}{\pi t_{exp}}}$	$k_c \propto D_{AB}^{1/2}$	t_{exp} unknown
Boundary-layer theory	$k_c = 0.664 \frac{D_{AB}}{L} \text{Re}_L^{1/2} \text{Sc}^{1/3}$	$k_c \propto D_{AB}^{2/3}$	Best way to scale k_c from one solute to another exposed to same hydrodynamic flow

Effect on D_{AB} may be used to scale mass transfer coefficients from one solute to another when they are exposed to the same hydrodynamic flows

Summary of models proposed for mass transfer coefficients

Mass Transport "Laws"

We now have 2 Mass Transport "laws"

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Predicts flux N_A and composition distributions, e.g. $x_A(x, y, z, t)$

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Since we predict N_A , we can also predict a mass xfer coeff k_y or k_c

Diffusion coefficients are **material** properties (see tables)

Linear-Driving-Force Model $|N_A| = k_y |x_{A,bulk} - x_A|$

Use: Combine with macroscopic species A mass balance
Predicts flux N_A but **not** composition distributions
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Facilitate combining resistances into overall mass xfer coeffs, K_L, K_G

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Mass Transport "Laws"

We now have 2 Mass Transport "laws"

Remaining Topics to round out our understanding of mass transport:

Fick's law of diffusion

D_{AB}

1. Since we predict N_A with Fick's law, we can also predict a mass transfer coefficients k_y or k_c *Relate k_c and D_{AB}*
2. 1D Unsteady models can be solved (if good at math)

Mass transfer coefficients

k_c

3. Combine with macroscopic species A mass balance
4. Are not material properties; rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations)
5. Facilitate combining resistances into overall mass transfer coefficients, K_L, K_G , to be used in modeling unit operations

Mass Transport "Laws"

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Unsteady Macroscopic Species A Mass Balance




Michigan Tech

CM3110
Transport II
Part II: Diffusion and Mass Transfer

2


Unsteady State
Solutions to
Diffusion Problems



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Unsteady State Mass Transport

Unsteady State Diffusion in a Semi-Infinite Slab



$$\frac{\partial c_A}{\partial t} = D_{AB} \left(\frac{\partial^2 c_A}{\partial z^2} \right)$$

Initial condition: $t = 0 \quad c_A = c_{A0} \quad \forall z$

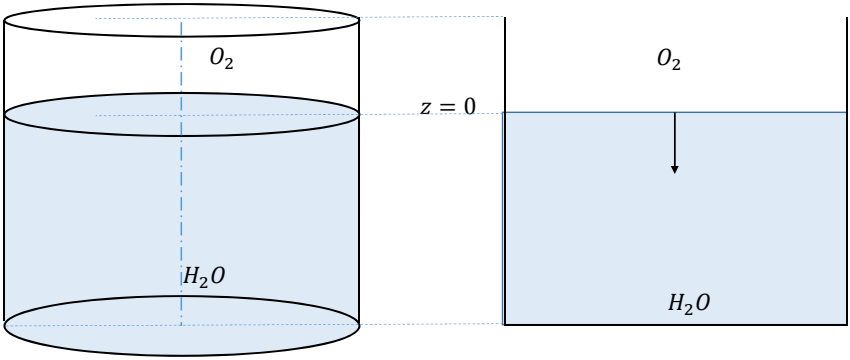
Boundary conditions:

$x = 0$	$c_A = c_{As}$	$t > 0$
$x = \infty$	$c_A = c_{A0}$	$\forall t$

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Unsteady State Mass Transport

Example: A very long, very large tank of water is suddenly exposed to oxygen atmosphere. Oxygen diffuses into the water. What is the concentration profile of the oxygen in the water as a function of time?

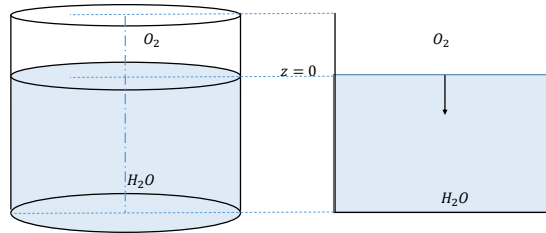


WRF, p534

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Unsteady State Mass Transport

Example: A very long, very wide tank of water is suddenly exposed to oxygen atmosphere. Oxygen diffuses into the water. What is the concentration profile of the oxygen in the water as a function of time?



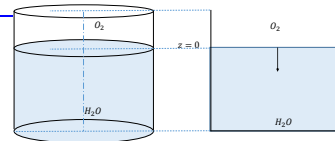
You try.

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Unsteady State Mass Transport

Unsteady State Diffusion in a Semi-Infinite Slab



$$\frac{\partial c_A}{\partial t} = D_{AB} \left(\frac{\partial^2 c_A}{\partial z^2} \right)$$

The "diffusion equation"

Initial condition: $t = 0 \quad c_A = c_{A0} \quad \forall z$

Boundary conditions:

$$x = 0 \quad c_A = c_{As} \quad t > 0$$

$$x = \infty \quad c_A = c_{A0} \quad \forall t$$

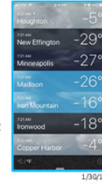
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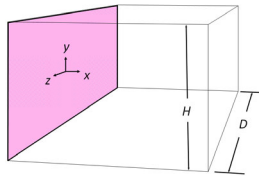
We've seen this mathematics problem before.

Example:
When will my pipes freeze?

The temperature has been 35°F for a while now, sufficient to chill the ground to this temperature for many tens of feet below the surface. Suddenly the temperature drops to -20°F. How long will it take for freezing temperatures (32°F) to reach my pipes, which are 8 ft under ground?

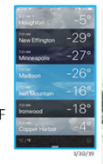


Develop a model:



Example:
When will my pipes freeze?

The temperature has been 35°F for a while now, sufficient to chill the ground to this temperature for many tens of feet below the surface. Suddenly the temperature drops to -20°F. How long will it take for freezing temperatures (32°F) to reach my pipes, which are 8 ft under ground?



Example 1: Unsteady Heat Conduction in a Semi-infinite solid

A very long, very wide, very tall slab is initially at a temperature T_0 . At time $t = 0$, the left face of the slab is exposed to a vigorously mixed gas at temperature T_1 . What is the time-dependent temperature profile in the slab?

Unsteady State Heat Transfer: Lecture 6 Earlier

Example: **Unsteady** Heat Conduction in a Semi-infinite solid

$H, D, \text{ very large}$

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Unsteady State Heat Transfer: Lecture 6 Earlier

Initial Condition:

$t < 0$
 $T = T_0$

$t < 0$
 $T = T_0$

Then,

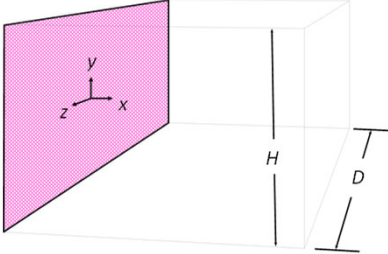
$t \geq 0$
 $T = T_1$

$t > 0$
 $T = T(x, t)$

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Unsteady State Heat Transfer: Lecture 6 Earlier

Example: Unsteady Heat Conduction in a Semi-infinite solid



Initial Condition:

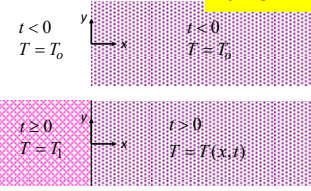
$t < 0$ $T = T_o$	y ↑ x →	$t < 0$ $T = T_o$
$t \geq 0$ $T = T_1$	y ↑ x →	$t > 0$ $T = T(x,t)$

You try.

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Unsteady State Heat Transfer: Lecture 6 Earlier

Unsteady State Heat Conduction in a Semi-Infinite Slab



$$\frac{\partial T}{\partial t} = \frac{k}{\rho \hat{C}_p} \left(\frac{\partial^2 T}{\partial x^2} \right) = \alpha \left(\frac{\partial^2 T}{\partial x^2} \right)$$

thermal diffusivity

$$\alpha \equiv \frac{k}{\rho \hat{C}_p}$$

Initial condition: $t = 0 \quad T = T_o \quad \forall x$

Boundary conditions:

$x = 0$	$\frac{q_x}{A} = -k \frac{dT}{dx} = h(T_1 - T)$	$t > 0$
$x = \infty$	$T = T_o$	$\forall t$

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Unsteady State Heat Transfer: Lecture 6

Unsteady State Heat Conduction in a Semi-Infinite Slab

Solution:

$$\frac{T - T_0}{T_1 - T_0} = \text{erfc } \zeta - e^{\beta(2\zeta + \beta)} \text{erfc}(\zeta + \beta)$$

$$\beta \equiv \frac{h\sqrt{\alpha t}}{k} \quad \zeta \equiv \frac{x}{2\sqrt{\alpha t}}$$

Earlier ...

$$Y \equiv \frac{(T_1 - T)}{(T_1 - T_0)}$$

$$1 - Y = \frac{(T - T_0)}{(T_1 - T_0)}$$

complementary error function of y
(a standard function in Excel)

error function of y

$$\text{erfc}(y) \equiv 1 - \text{erf}(y)$$

$$\text{erf}(y) \equiv \frac{2}{\sqrt{\pi}} \int_0^y e^{-(y')^2} dy'$$

- Geankoplis 4th ed., eqn 5.3-7, page 363
- WRF, eqn 18-21, page 286

thermal diffusivity $\alpha \equiv \frac{k}{\rho c_p}$

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Unsteady State Mass Transport

The mathematics of unsteady state mass transfer is, in many cases, **directly analogous** to problems in unsteady state heat transfer.

We do not need to solve the differential equations again; just re-use the solutions, including Heissler charts. *Provided BC and IC are the same.*

Unsteady State Mass Transport

Unsteady State Diffusion in a Semi-Infinite Slab

$$\frac{\partial c_A}{\partial t} = D_{AB} \left(\frac{\partial^2 c_A}{\partial z^2} \right)$$

Initial condition: $t = 0 \quad c_A = c_{A0} \quad \forall z$

Boundary conditions:

$$x = 0 \quad c_A = c_{As} \quad t > 0$$

$$x = \infty \quad c_A = c_{A0} \quad \forall t$$

Unsteady State Heat Transfer: Lecture 6

Unsteady State Heat Conduction in a Semi-Infinite Slab

$$\frac{\partial T}{\partial t} = \frac{k}{\rho \hat{c}_p} \left(\frac{\partial^2 T}{\partial x^2} \right) = \alpha \left(\frac{\partial^2 T}{\partial x^2} \right)$$

thermal diffusivity $\alpha \equiv \frac{k}{\rho \hat{c}_p}$

Initial condition: $t = 0 \quad T = T_0 \quad \forall x$

Boundary conditions:

$$x = 0 \quad \frac{q_x}{A} = -k \frac{dT}{dx} = h(T_1 - T) \quad t > 0$$

$$x = \infty \quad T = T_0 \quad \forall t$$

(For the pipe-freezing problem we did the Newton's law of cooling BC case, but the soln with temperature BCs is in the literature too.)

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Unsteady State Mass Transport

The mathematics of unsteady state **mass** transfer is, in many cases, **directly analogous** to problems in unsteady state **heat** transfer.

We do not need to solve the differential equations again; we can just re-use the solutions. (including Heissler charts)

FIGURE 5.3-10. Charts for determining the temperature at the center of a sphere for unsteady-state heat conduction. (From H. P. Heissler, Trans. A.S.M.E., 80, 217 (1958), with permission.)

From Geankoplis, 4th edition, page 374

Conduction of Heat in Solids

SECOND EDITION

OXFORD
AT THE CLARENDON PRESS

H. S. CARSLAW and
J. C. JAEGER

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Unsteady State Mass Transport

O₂ Diffusion Solution:

The oxygen concentration as a function of time and depth into the water is given by:

$$\frac{c_{As} - c_A}{c_{As} - c_{A0}} = \operatorname{erfc}\left(\frac{z}{2\sqrt{D_{AB}t}}\right) = \operatorname{erfc}\zeta$$

$$\zeta \equiv \frac{z}{2\sqrt{D_{AB}t}}$$

Unsteady State Mass Transport

Unsteady State Diffusion in a Semi-Infinite Slab

$$\frac{\partial c_A}{\partial t} = D_{AB} \left(\frac{\partial^2 c_A}{\partial z^2} \right)$$

Initial condition: $t = 0 \quad c_A = c_{A0} \quad \forall z$

Boundary conditions:

$x = 0 \quad c_A = c_{As} \quad t > 0$

$x = \infty \quad c_A = c_{A0} \quad \forall t$

Oxygen Diffusion

time, s:
— 1
— 2
— 5
— 10
— 20
— 50
— 100
— 200
— 500

(arbitrary numbers)

D_{AB} = 0.001 cm²/s
c_{As} = 0.1 mol/cm³
c_{A0} = 0.005 mol/cm³

WRF, p534

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Unsteady State Mass Transport

O₂ Diffusion Solution:

The oxygen concentration as a function of time and depth into the water is given by:

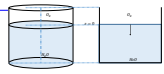
$$\frac{c_{As} - c_A}{c_{As} - c_{A0}} = \operatorname{erfc}\left(\frac{z}{2\sqrt{D_{AB}t}}\right) = \operatorname{erfc}\zeta$$

$$\zeta \equiv \frac{z}{2\sqrt{D_{AB}t}}$$

This solution was a resource in the Danckwerts model for mass transfer; the short penetration time meant that the diffusion direction looked "infinite."

Unsteady State Mass Transport

Unsteady State Diffusion in a Semi-Infinite Slab



$$\frac{\partial c_A}{\partial t} = D_{AB} \left(\frac{\partial^2 c_A}{\partial z^2} \right)$$

Initial condition: $t = 0 \quad c_A = c_{A0} \quad \forall z$

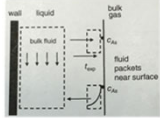
Boundary conditions:

$$x = 0 \quad c_A = c_{As} \quad t > 0$$

$$x = \infty \quad c_A = c_{A0} \quad \forall t$$

Mass Transport "Laws"

Another physical picture associated with penetration theory is "surface renewal" (Danckwerts)



- Turbulent flow
- Diffusing species only penetrates a short distance
- Due to chem rxn or short time of contact, t_{exp}
- Model as unsteady state molecular transport
- Dankwerts: bulk motion brings fresh liquid eddies from interior to the surface
- At the surface A is transferred as though it were stagnant and in finitely deep
- Works for falling film

$$k_c = \sqrt{\frac{4D_{AB}}{\pi t_{exp}}}$$

WRF, p534 61

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Unsteady State Mass Transport

Summary of Unsteady Diffusion:

- ➔ The microscopic balances of energy and mass of species A are quite similar mathematically:

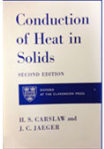
$$\left(\frac{\partial T}{\partial t} + \underline{v} \cdot \nabla T \right) = \alpha \nabla^2 T + S_e$$

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

- ➔ Some of the boundary conditions are also similar, e.g.:

$t = 0$	T or $\omega_A =$ known value
$z = 0, \infty$	T or $\omega_A =$ known value
$z = 0, \infty$	$\frac{\partial T}{\partial z}$ or $\frac{\partial \omega_A}{\partial z} =$ known value
$z = z_1$	$\frac{\partial T}{\partial z}$ or $\frac{\partial \omega_A}{\partial z} =$ linear driving force expression (h or k_c)

- ➔ Literature results for heat transfer can be repurposed for species A mass transfer
- ➔ Intuition for heat transfer is plausible to use for species A mass transfer



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Mass Transport "Laws"

We now have 2 Mass Transport "laws"

Remaining Topics to round out our understanding of mass transport:

Fick's law of diffusion

D_{AB} {

1. Since we predict \bar{N}_A with Fick's law, we can also predict a mass transfer coefficient k_y or k_c *Relate k_c and D_{AB}*
2. 1D Unsteady models can be solved (if good at math) *Solutions are analogous to heat transfer*

Mass transfer coefficients

k_c {

3. **Combine with macroscopic species A mass balance**
4. Are not material properties; rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations)
5. Facilitate combining resistances into overall mass transfer coefficients, K_L, K_G , to be used in modeling unit operations

Mass Transport "Laws"

We now have 2 Mass Transport "laws" Transport coefficient

Fick's Law of Diffusion $\bar{N}_A = x_A(\bar{N}_A + \bar{N}_B) - cD_{AB}\nabla x_A$

Use: Combine with microscopic species A mass balance
Predicts flux \bar{N}_A and composition distributions, e.g. $x_A(x, y, z, t)$

1D Steady models can be solved

1D Unsteady models can be solved (if good at math) ②

2D steady and unsteady models can be solved by Comsol

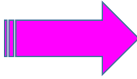
Since we predict \bar{N}_A , we can also predict a mass xfer coeff k_y or k_c ①

Diffusion coefficients are **material** properties (see tables)

Linear-Driving-Force Model $|N_{A,i}| = k_y |y_{A, bulk} - y_{A,i}|$

Use: Combine with macroscopic species A mass balance ③
Predicts flux \bar{N}_A , but **not** composition distributions
May be used as a boundary condition in microscopic balances
Mass-transfer-coefficients are **not material properties**
Rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations) ④
Facilitate combining resistances into overall mass xfer coeffs, K_L, K_G ⑤

Keep cranking at the list



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