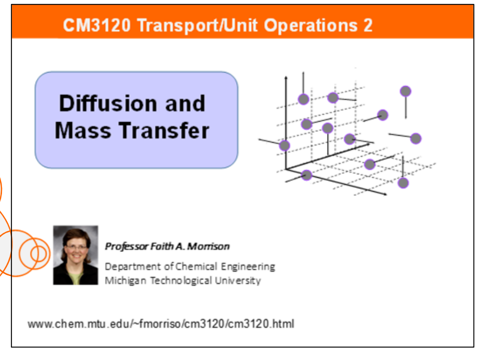

Where are we?

Time for a recap.

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

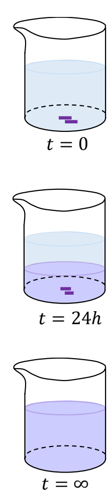
Mixtures

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

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- Includes *all* mechanisms
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- Linear-driving-force model,
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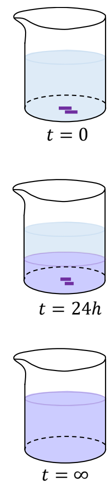
Haven't actually talked about this yet



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Diffusion/Mass Transfer Recap and Planning

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

Modeling:

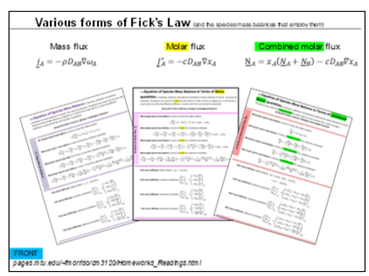
Microscopic species A mass balance
(continuum modeling tricky with mixtures; also issues of units, (mass versus moles) and reference coordinates)

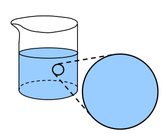
- Four fluxes $\underline{N}_A, \underline{J}_A^*, \underline{n}_A, \underline{j}_A$
- Three summary sheets using $\underline{N}_A, \underline{J}_A^*, \underline{j}_A$

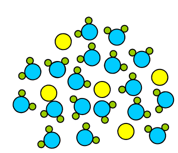
Fick's law (diffusion)

- 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 $k_{various\ designations}$







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Diffusion/Mass Transfer Recap and Planning

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

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

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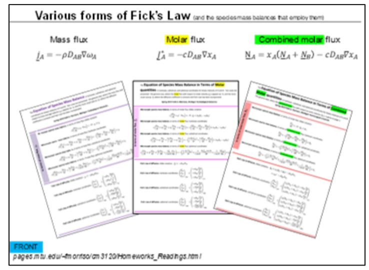
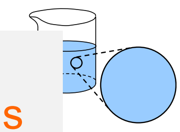
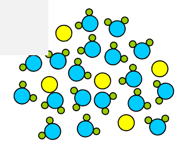
Linear-driving-force model (mass transfer; analogous to Newton's law of cooling)—mass transfer coefficient $k_{various\ designations}$

Have not touched this yet







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Diffusion/Mass Transfer Recap and Planning

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

Modeling:

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- Fou
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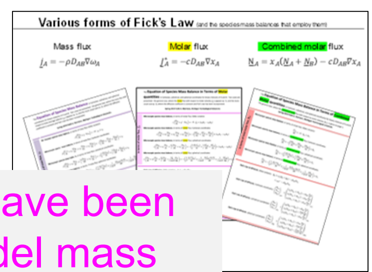
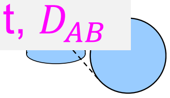
  $\underline{N}_A, \underline{J}$

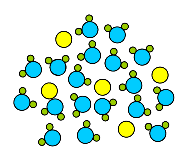
Up to now, we have been learning to model mass transfer using Fick's law and the diffusion coefficient, D_{AB}

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 $k_{various\ designations}$







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Diffusion/Mass Transfer Recap and Planning

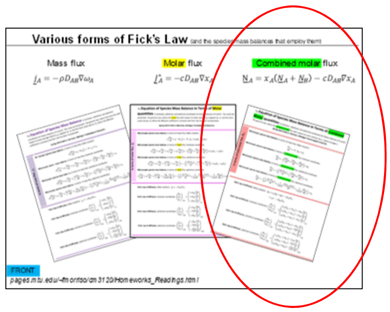
Recap:
Diffusion/Mass Transfer (so far, and beyond)

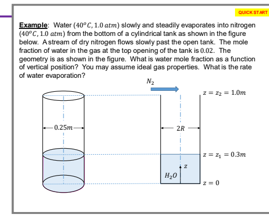
We did a Quick Start:

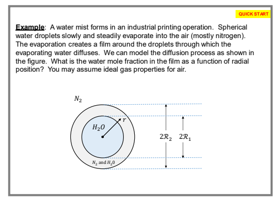
$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

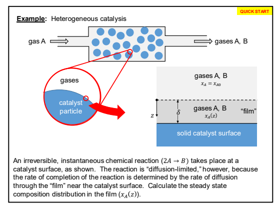
$$\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$$

Learning to use the microscopic species A balance









and later,  **Cycled Back:**

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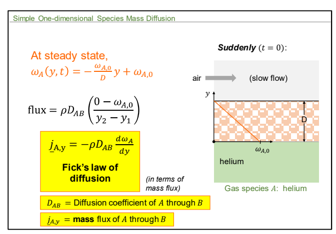
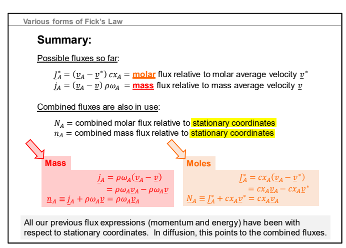
Diffusion/Mass Transfer Recap and Planning

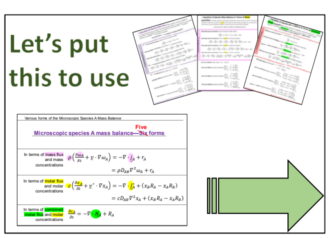
Recap:
Diffusion/Mass Transfer (so far, and beyond)

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







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Diffusion/Mass Transfer Recap and Planning

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

Problems Solved

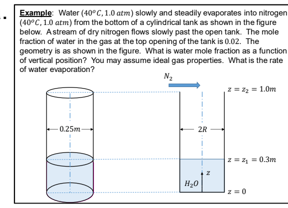
(1D), Steady:

a. Unimolecular mass transfer
b. Heterogeneous chemical reaction
c. Equimolar counter diffusion
d. Homogeneous chemical reaction

Applied to Unit Operations:

a. Evaporation (tank)
b. Catalytic reactors
c. Distillation
d. Absorption

a.



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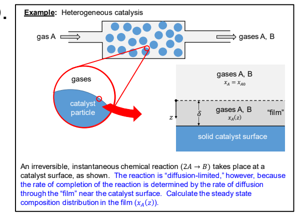

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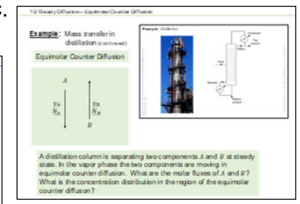

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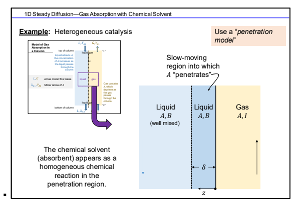

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Diffusion/Mass Transfer Planning

... and beyond

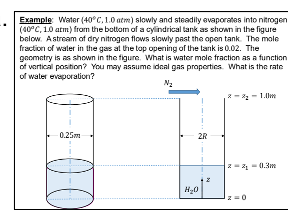
For all these problems we used the $\underline{N}_A$ approach:

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

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

Why?

a.



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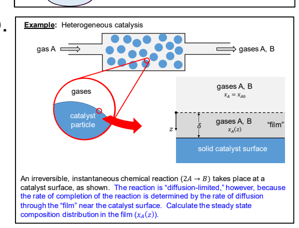

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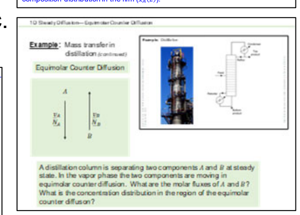
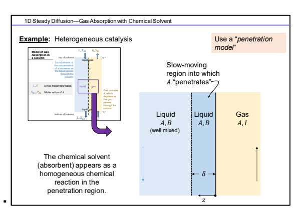


d.



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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.

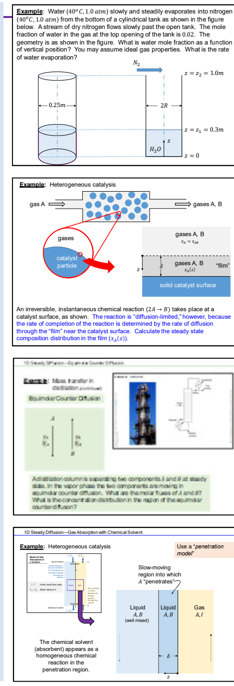
In these problems, convection was caused by diffusion only.

a. $N_{B,z} = 0$

b. $N_{B,z} = -\frac{1}{2}N_{A,z}$

c. $N_{A,z} + N_{B,z} = 0$

d. $N_{B,z} = 0$



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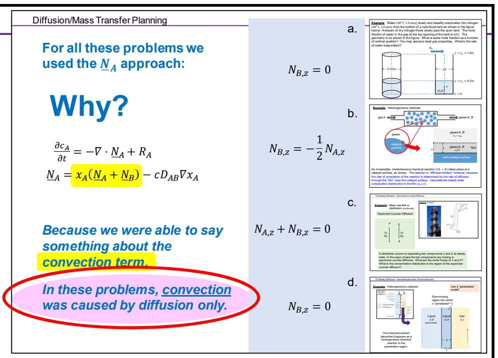
Diffusion/Mass Transfer Planning



Microscopic species A mass balance

convection

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

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

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

combined convection and diffusion

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

Yet, this includes most situations.

?

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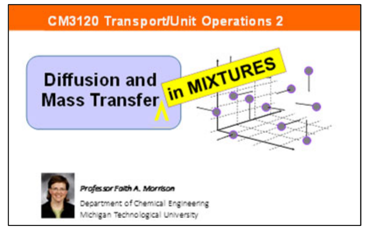
Diffusion/Mass Transfer Planning

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



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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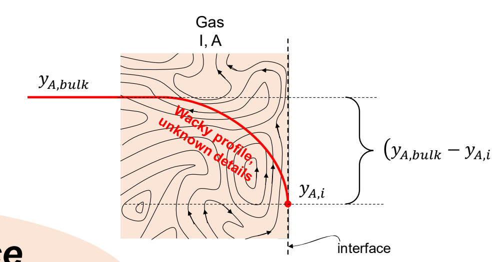
Linear Driving Force Model for Mass Transfer

Michigan Tech

CM3110
Transport II
Part II: Diffusion and Mass Transfer



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

Linear Driving Force Model for Mass Transfer

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

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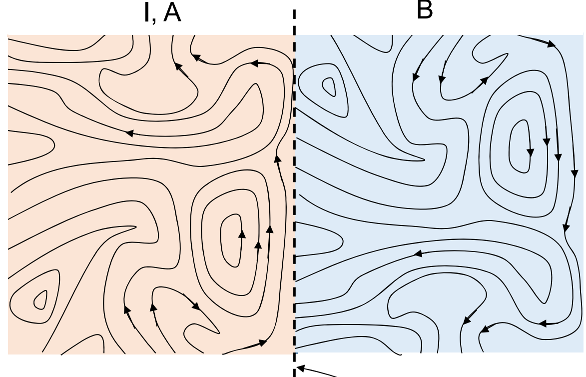
Bulk convection present- Linear-driving-force model

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**



Bulk flow is present.

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

?

WRF, Ch29 p 596

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Bulk convection present- Linear-driving-force model

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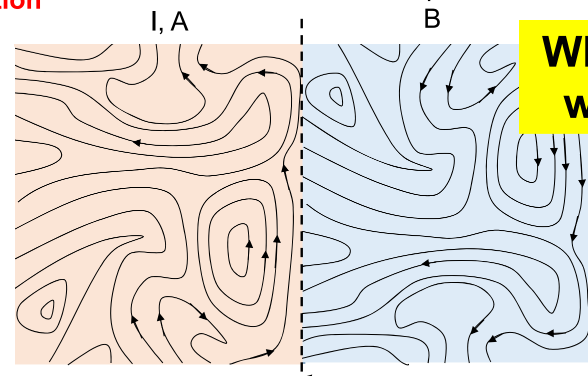

What can we do?

Bulk flow is present.

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

?

WRF, Ch29 p 596

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Bulk convection present- Linear-driving-force model

Remember *Newton's law of cooling*?

What about this case?

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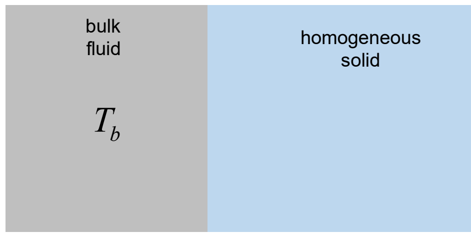
Example 2: Heat flux in a rectangular solid – *Fluid* BC

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

Remember *Newton's law of cooling*?

What about this case?

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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

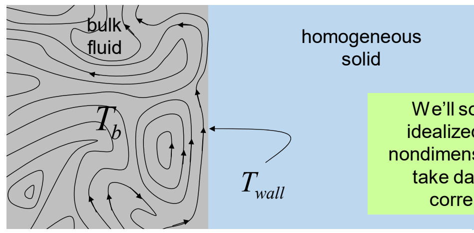
Remember *Newton's law of cooling*?

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

CM3110

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!

$T_b \neq T_{wall}$

$\underline{v}(x,y,z) \neq 0$

What is the flux at the wall?

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Bulk convection present- Linear-driving-force model

Remember *Newton's law of cooling*?

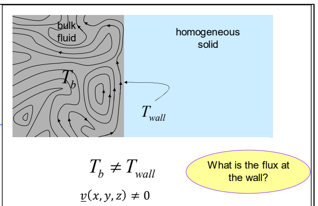
= **linear-driving-force model**

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

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

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

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.

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

***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.

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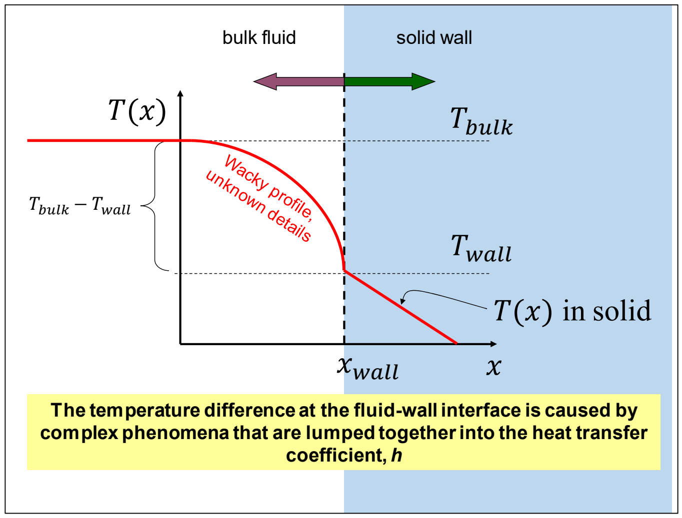
Bulk convection present- Linear-driving-force model

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.



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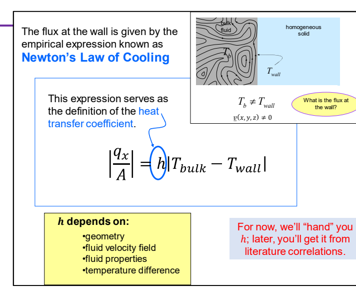
Bulk convection present- Linear-driving-force model

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.



We can do the same with mass transfer coefficient:

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

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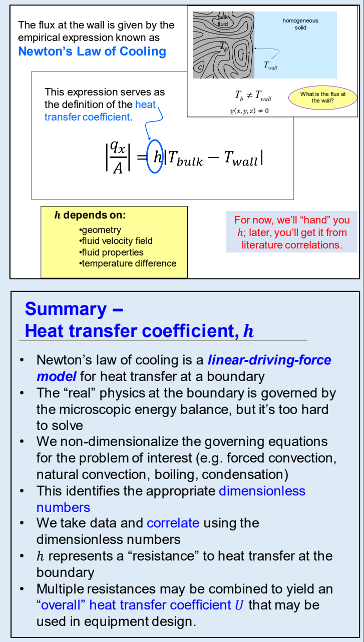
Bulk convection present- Linear-driving-force model

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

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

(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)

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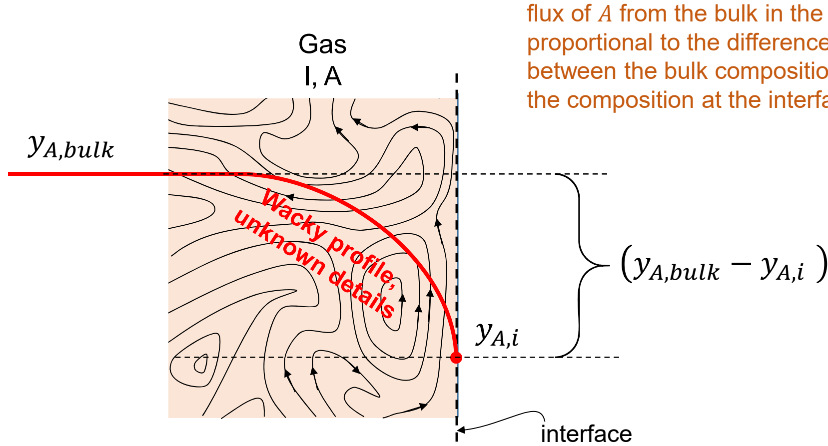
Bulk convection present- Linear-driving-force model

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.

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

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

WRF, Ch29 p 596

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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:

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

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

(sometimes called "diffusion velocity")

(gases) $$N_A = \frac{k_c}{RT}\left(p_{A,bulk} - p_{A,i}\right)$$

WRF, Ch29 p 596

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Bulk convection present- Linear-driving-force model

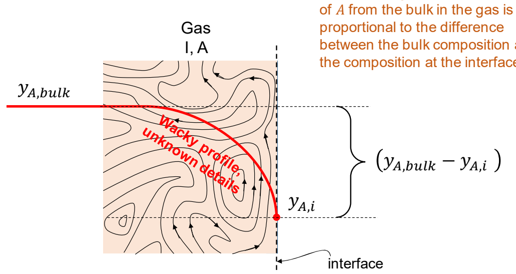
With this method, we do not model the details of the diffusion and convection in the gas.

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

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

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

WRF, Ch29 p 596

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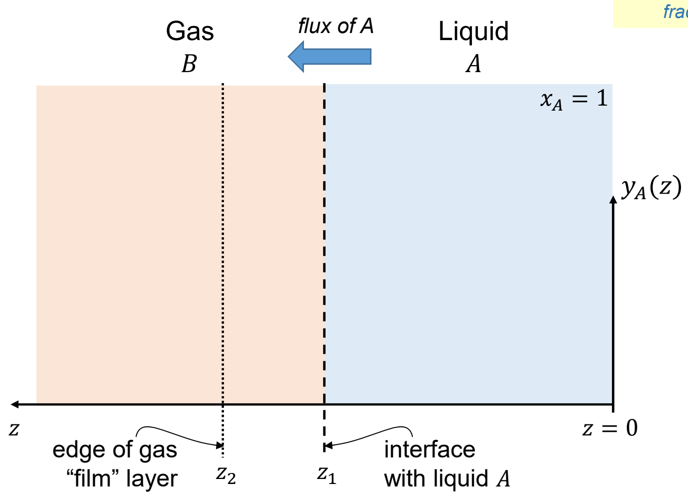
Bulk convection present- Linear-driving-force model

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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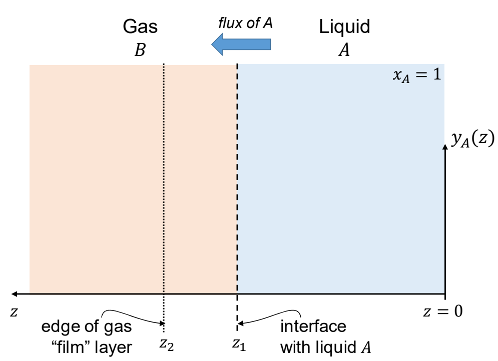
Bulk convection present- Linear-driving-force model

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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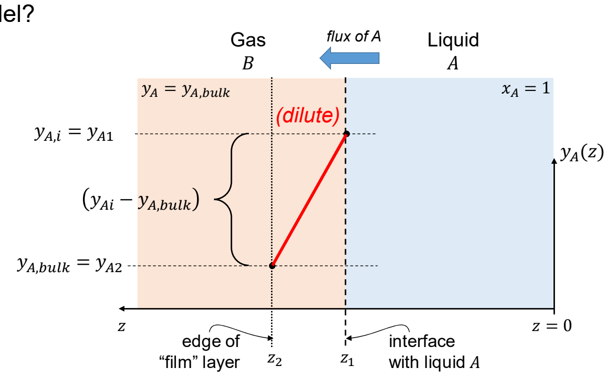
Bulk convection present- Linear-driving-force model

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:

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

$$y_{Blm} \equiv \frac{(y_{B2} - y_{B1})}{\ln\left(\frac{y_{B2}}{y_{B1}}\right)}$$

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

Film model prediction for mass-transfer coefficient

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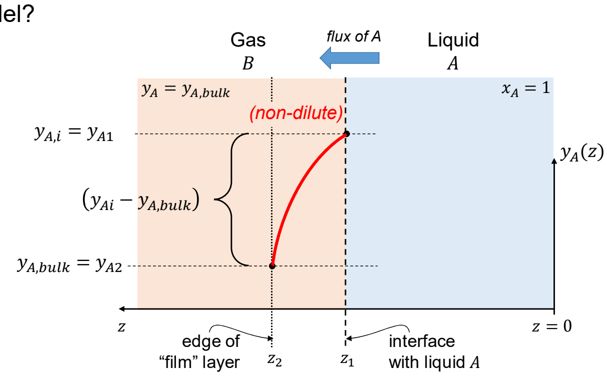
Bulk convection present- Linear-driving-force model

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?



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

Film model prediction for mass-transfer coefficient

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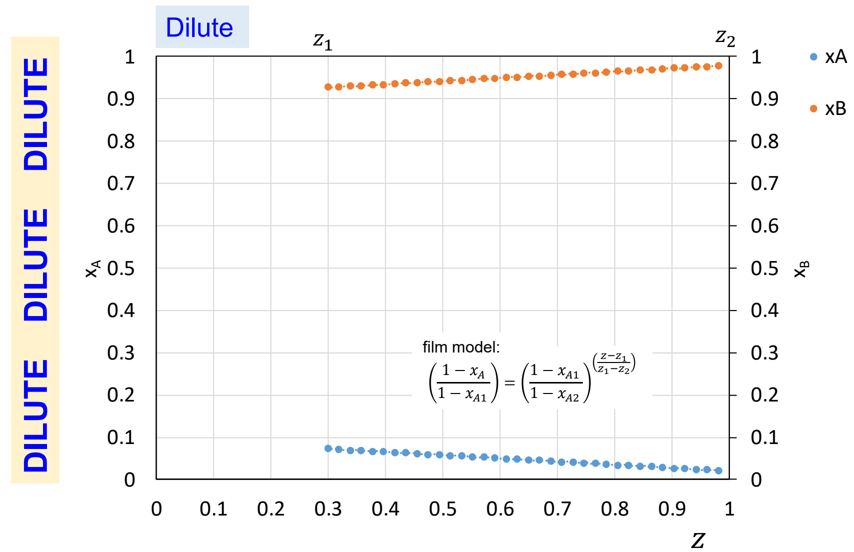
Bulk convection present- Linear-driving-force model

(see Example 1)

The film model for $x_{A1} = 0.0728$, $x_{A2} = 0.02$
$0.3 \leq z \leq 1.0$



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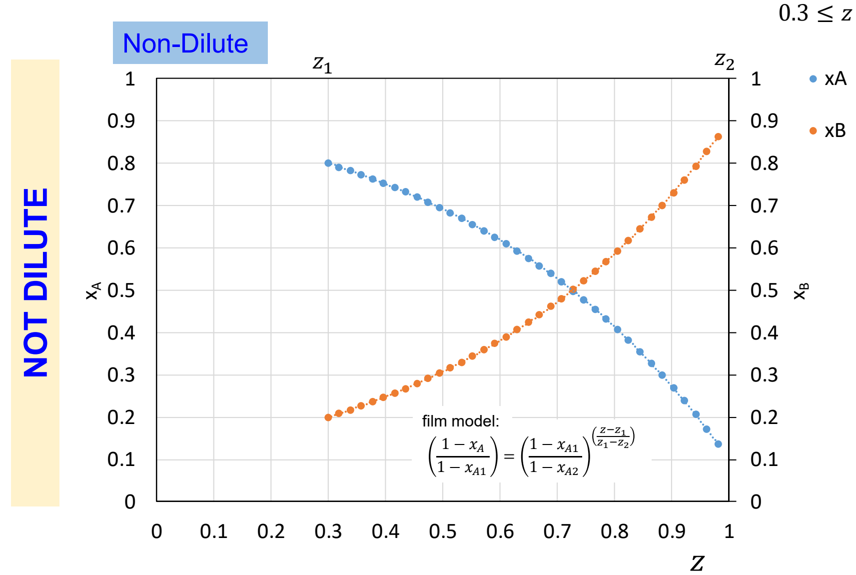
Bulk convection present- Linear-driving-force model

The film model for $x_{A1} = 0.8000$, $x_{A2} = 0.10$
$0.3 \leq z \leq 1.0$



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Mass-transfer coefficient for film model

We used mole fraction units:

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

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

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

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

…

$$k_c = \frac{PD_{AB}}{\delta\left(P_{B_{lm}}\right)}$$

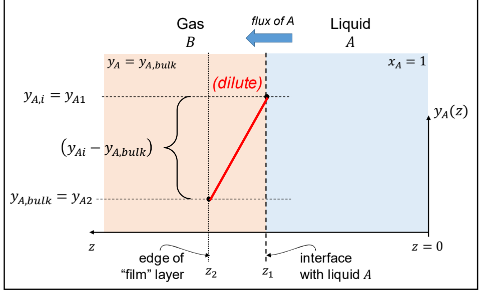
Film model prediction for mass transfer coefficient

WRF eqn 26-9

film model

$$k_c \propto D_{AB}$$

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?



WRF, Ch26 p 492

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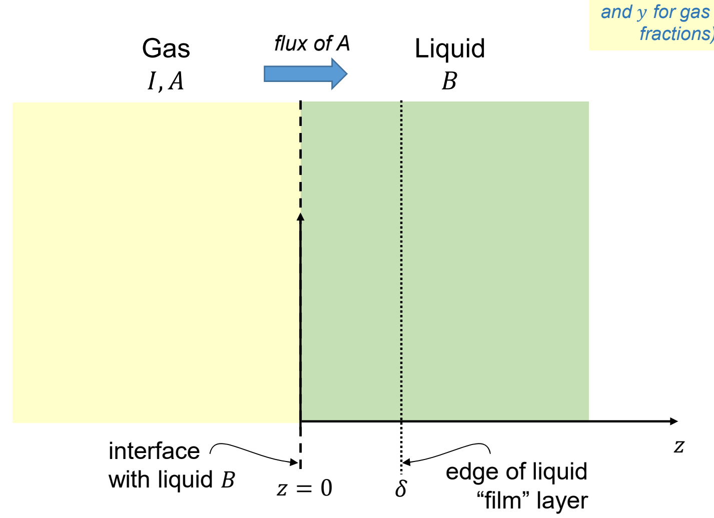
Example: The penetration model of 1D steady diffusion yields a composition distribution and an expression for the flux. What is the mass-transfer coefficient in the penetration model?

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



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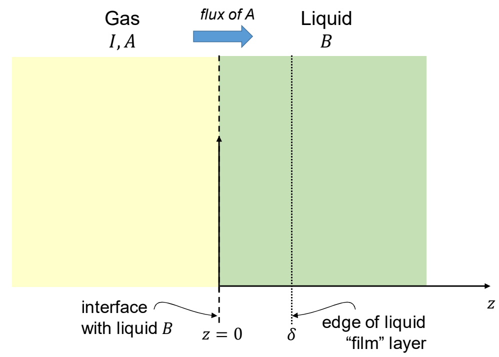
Bulk convection present- Linear-driving-force model

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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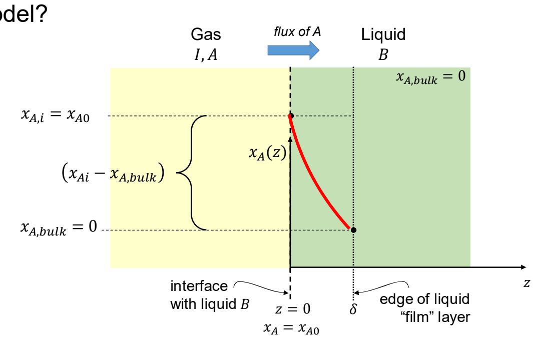
Bulk convection present- Linear-driving-force model

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:

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

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

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

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

penetration model

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

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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 $\underline{N}_A$ <u>and</u> 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 <u>not</u> composition distributions
May be used as a boundary condition in microscopic balances
Mass-transfer-coefficients are ***<u>not</u> 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"

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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
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) (2)
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 (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 (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***
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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Mass Transport "Laws"

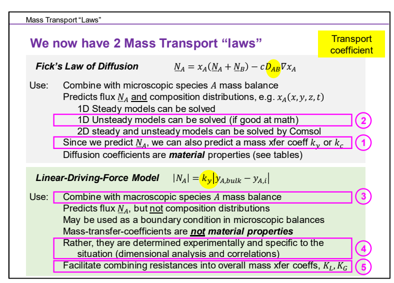
We now have 2 Mass Transport "laws"

Remaining Topics to round out our understanding of mass transport:

Fick's law of diffusion

D_{AB}

1. Since we predict $\underline{N}_A$ with Fick's law, we can also predict a mass transfer coefficients 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

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We now have 2 Mass Transport "laws"

Remaining Topics to round out our understanding of mass transport:

Fick's law of diffusion

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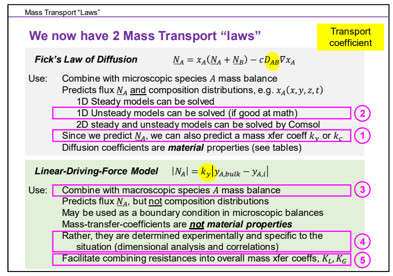

Mass transfer coefficients

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.

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Michigan Tech

CM3110
Transport II
Part II: Diffusion and Mass Transfer

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	$k_c = 0.664\frac{D_{AB}}{L}\mathrm{Re}_L^{1/2}\,\mathrm{Sc}^{1/3}$	$k_c \propto D_{AB}^{2/3}$

Predicting Mass-Transfer Coefficients

From solutions to the microscopic species A mass balance

1

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Michigan Technological University

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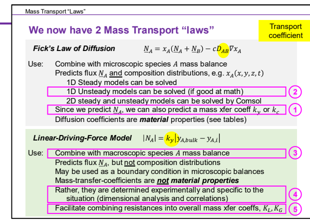
Mass Transport "Laws"


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. $x_A(x,y,z,t)$
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 $\underline{N}_A$, 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 (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***
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)

(1) Since we predict $\underline{N}_A$ with Fick's law, we can also predict a mass transfer coefficients k_y or k_c with Fick's law

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

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

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

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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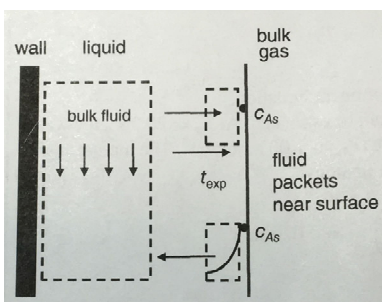
Mass Transport "Laws"

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



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

- 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

WRF, Ch28 p 584

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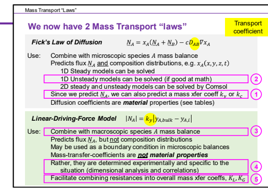
Mass Transport "Laws"

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***

Table 28.1 Models for convective mass-transfer coefficients (dilute systems)

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	$k_c = 0.664\frac{D_{AB}}{L}Re_L^{1/2}\,Sc^{1/3}$	$k_c \propto D_{AB}^{2/3}$	Best way to scale k_c from one solute to another exposed to same hydrodynamic flow

Summary of ***models*** proposed for mass transfer coefficients

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

WRF, Ch28 p 586

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Mass Transport "Laws"

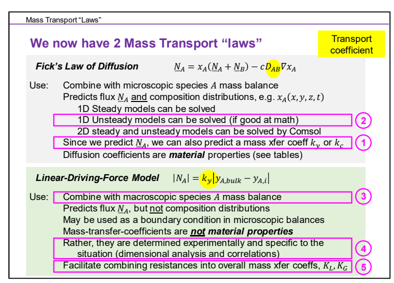
We now have 2 Mass Transport "laws"

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

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Unsteady Macroscopic Species A Mass Balance

Michigan Tech

CM3110
Transport II
Part II: Diffusion and Mass Transfer

Unsteady State Solutions to Diffusion Problems

2

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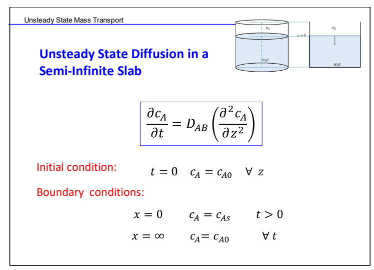
Department of Chemical Engineering
Michigan Technological University



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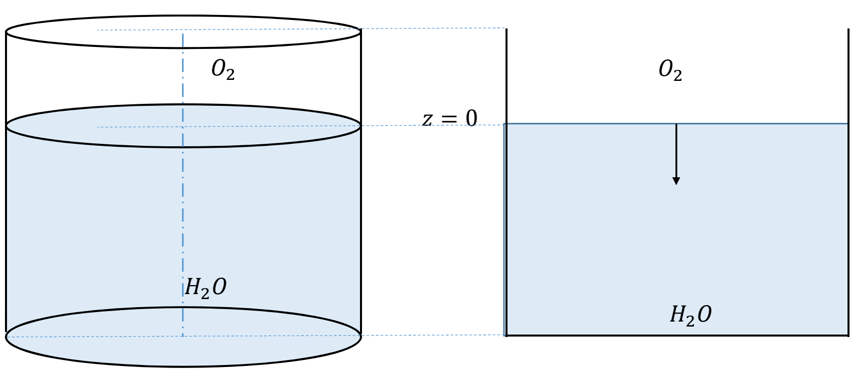
Unsteady State Mass Transport

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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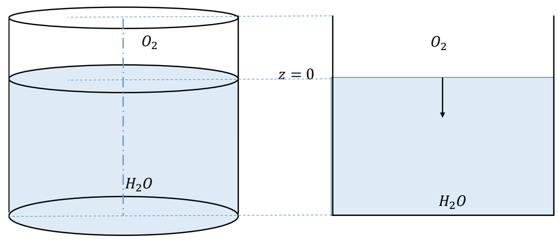
Unsteady State Mass Transport

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.

WRF, p534

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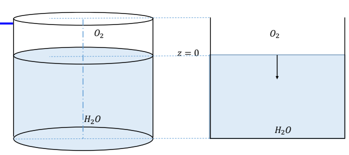
Unsteady State Mass Transport



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:

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

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

WRF, p534

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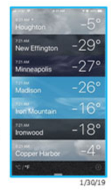
Unsteady State Heat Transfer: Lecture 6

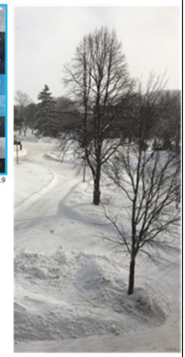
Earlier ….

We've seen this mathematics problem before.

Example:
When will my pipes freeze?

The temperature has been 35ºF 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 -20ºF. How long will it take for freezing temperatures (32ºF) to reach my pipes, which are 8 *ft* under ground?





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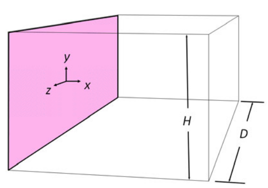
Unsteady State Heat Transfer: Lecture 6

Earlier ….

Develop a model:



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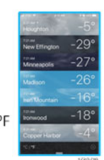

***Example 1:* Unsteady Heat Conduction in a Semi-infinite solid**

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?

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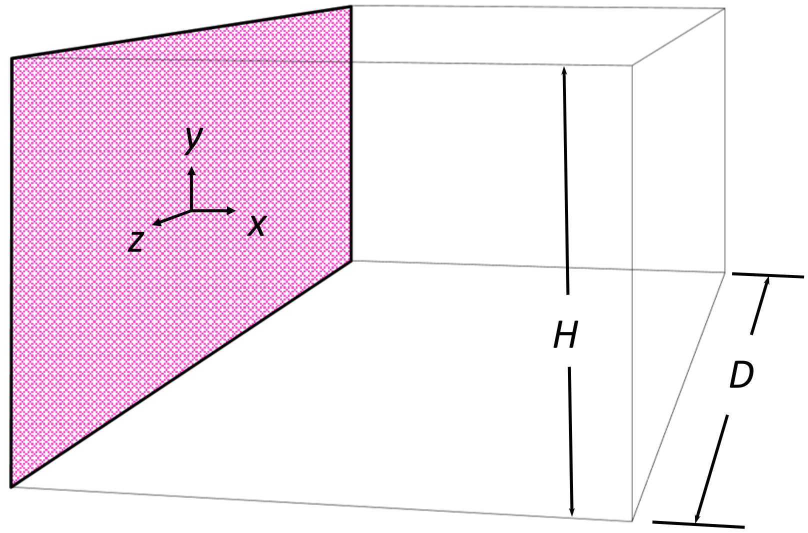
Earlier ….

Example: Unsteady Heat Conduction in a Semi-infinite solid



H, D, very large

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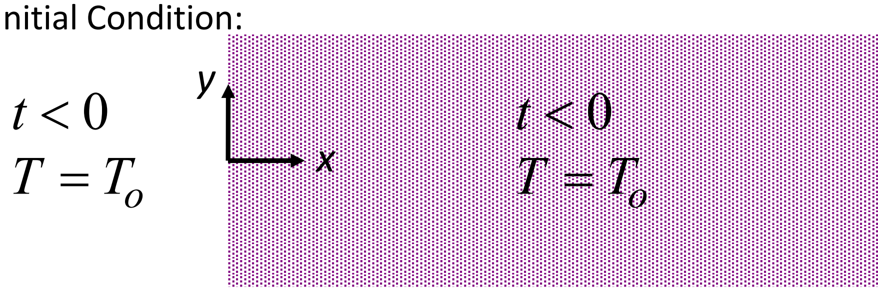
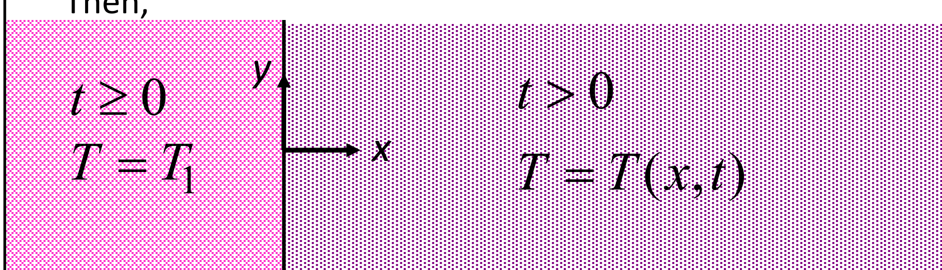
Earlier ….

Initial Condition:



Then,



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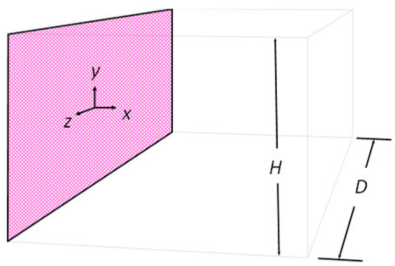
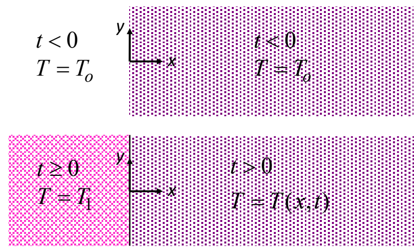
Unsteady State Heat Transfer: Lecture 6

Earlier ....

Example: Unsteady Heat Conduction in a Semi-infinite solid



Initial Condition:



You try.

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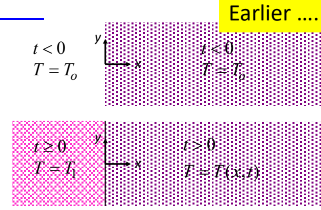
Unsteady State Heat Transfer: Lecture 6

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

Boundary conditions:

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

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

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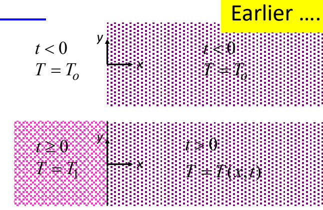
Unsteady State Heat Transfer: Lecture 6

Earlier ....

Unsteady State Heat Conduction in a Semi-Infinite Slab



Solution:

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

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

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

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

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

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

error function of y

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

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

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

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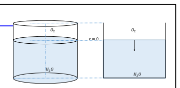
Unsteady State Mass Transport

The mathematics of unsteady state <u>mass</u> transfer is, in many cases, directly analogous to problems in unsteady state <u>heat</u> 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: $t=0 \quad c_A = c_{A0} \quad \forall\, z$

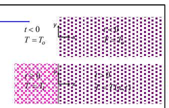
Boundary conditions:

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

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

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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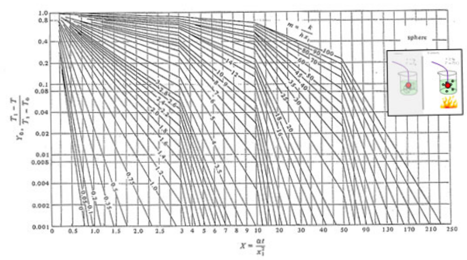
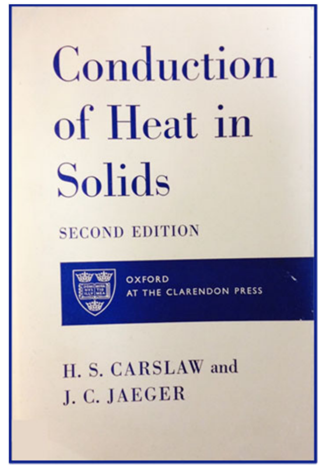
Unsteady State Mass Transport

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)



From Geankoplis, 4th edition, page 374



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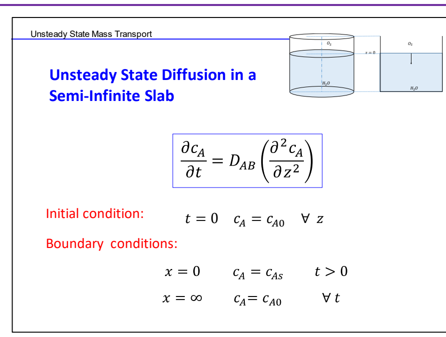
Unsteady State Mass Transport

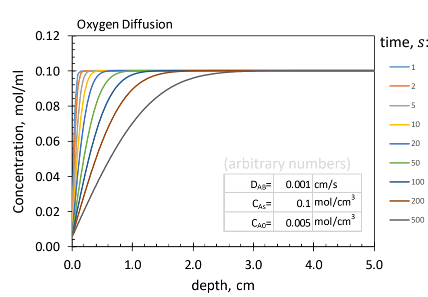
O_2 Diffusion Solution:

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

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

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





WRF, p534

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Unsteady State Mass Transport

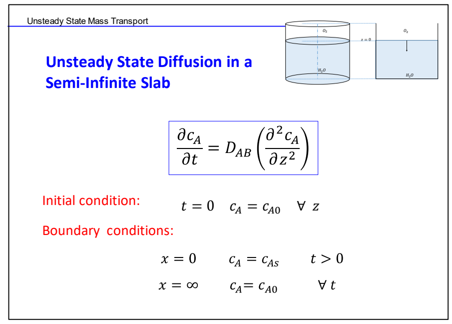
O_2 Diffusion Solution:

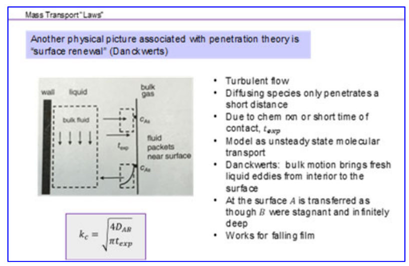
The oxygen concentration as a function of time and depth into the water is given by:

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

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

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





WRF, p534

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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 ω_A = known value
$z = 0, \infty$	T or ω_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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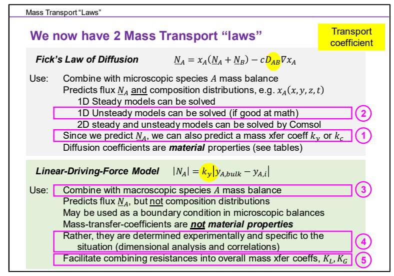
Mass Transport "Laws"

We now have 2 Mass Transport "laws"

Remaining Topics to round out our understanding of mass transport:


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. $x_A(x, y, z, t)$
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 $\underline{N}_A$, 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 (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***
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)

Fick's law of diffusion

D_{AB}

1. ✓ Since we predict $\underline{N}_A$ 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) *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

Keep cranking at the list

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