CM3120: Module 4

Diffusion and Mass Transfer II

I. Classic diffusion and mass transfer: d) EMCD
II. Classic diffusion and mass transfer: e) Penetration model
III. Unsteady macroscopic species A mass balances (Intro)
IV. Interphase species A mass transfers—To an interface—k_x, k_c, k_p
V. Unsteady macroscopic species A mass balances (Redux)
VI. Interphase species A mass transfers—Across multiple resistances—K_L, K_G
VII. Dimensional analysis
VIII. Data correlations

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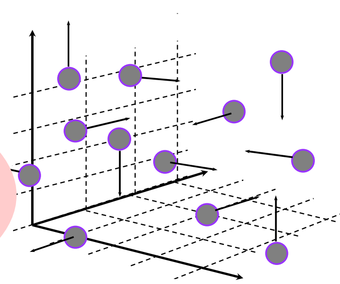
CM3120: Module 4

Module 4 Lecture IV

Interphase Transfers at Boundaries

(film mass transfer coefficients)



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

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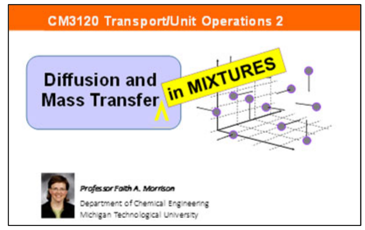
Interphase transfers at boundaries

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 the microscopic balance and **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 (such as in real, macroscopic devices), we need another approach.

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Unsteady Macroscopic Species A Mass Balance

Example 6—Revisited

In the previous lecture we tried to model an absorber.

We hit a road block: no way to quantify species A moving between phases

Let's return to that practical problem

Example 6: Height of a packed bed absorber

How can we use mass transfer to design a packed bed gas absorber to achieve a desired separation?

(started in Module 4, Lecture III)

BSL2 p742

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Modeling practical devices involving mass transfer

Example 6: Height of a packed bed absorber

How can we use mass transfer to design a packed bed gas absorber to achieve a desired separation?

Example 6 is presented as a series of **linked examples** that navigate around apparent "dead ends" in modeling mass-transfer units

LECTURES

Identify a question	Invent something	Try to use it
✓ 1. How can we model a large, practical device dependent on mass transfer? **III**	✓ 1. Apply the species A mass balance to a macroscopic C.V. **III**	✓ 1. Lack a system to account for A going between phases **PAUSE III**
2. How an we account for A going between phases? **IV**	2. Invent k_x through linear driving force (LDF) model **IV**	2. Gets A *to* the boundary, but not *across* **PAUSE V**
3. How can we improve LDF model to cross the boundary (bulk-to-bulk transfer)? **VI**	3. Write LDF in both phases and combine to create overall effect of multiple resistances **VI**	3. Working, but can we devise a convenient shorthand? **PAUSE VI**
4. Can we model a large, practical device, incorporating K_L, K_G to account for mass xfer between phases? **VI**	4. Yes **VI**	

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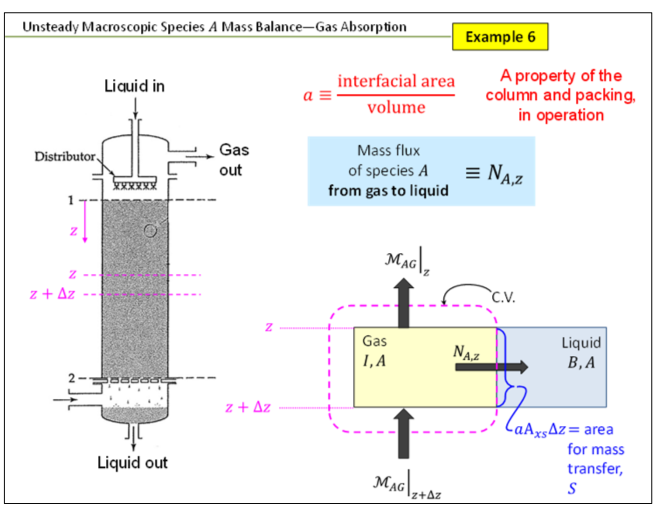
Film mass transfer coefficients, k_x, k_c, k_p

We chose a macroscopic C.V. and balanced species A.



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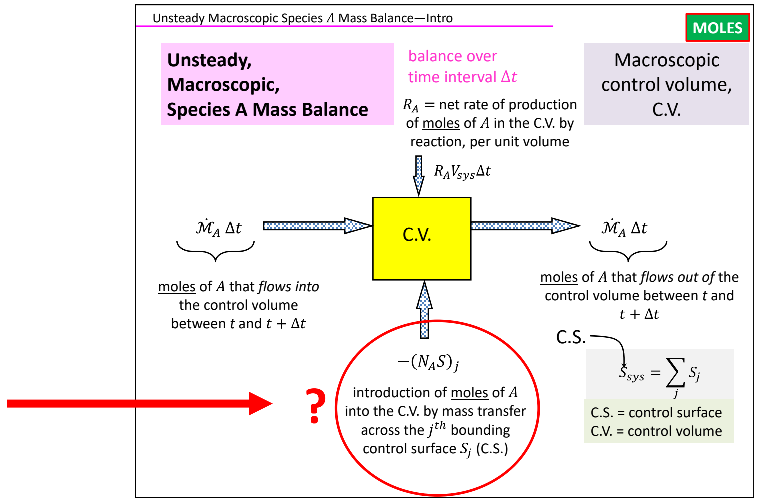
Film mass transfer coefficients, k_x, k_c, k_p

The macroscopic, unsteady, species A mass balance needs a way to include mass transfer across the control surfaces



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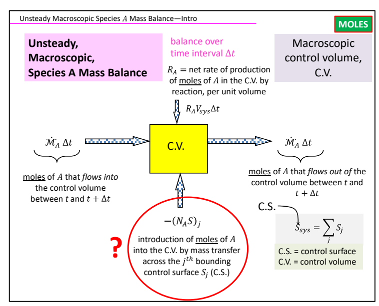
Film mass transfer coefficients, k_x, k_c, k_p



The solution is analogous to what we did in heat transfer: A **linear driving force model** like Newton's law of cooling. That "law" was invented because the turbulence in the fluid phase was too complicated to allow Fourier's law/temperature gradient to account for the heat transfer alone.

In mass-transfer unit operations, the **turbulence** in the fluid and gas phases are also too complicated to let Fick's law/species A concentration gradient account for the mass transfer alone.

Also, since mass-transfer devices are driven by **chemical affinities** (chemical potential), concentration gradients alone will not capture some of the most important mass transfer.

We start by defining the **mass-transfer law** (analogous to Newton's law of cooling) that will allow us to quantify mass transfer to (and from) macroscopic control volumes.

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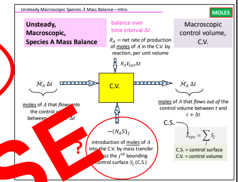
Let's keep this example on **PAUSE** as we develop the mass-transfer model we need

Film mass transfer coefficients, k_y, k_c, k_x

The solution is analogous to what we did in heat transfer: A **linear driving force model** like Newton's law of cooling. That "law" was invented because the turbulence in the fluid phase was too complicated to allow Fourier's law/temperature gradient to account for the heat transfer alone.



PAUSE

In mass-transfer unit operations, the **turbulence** in the fluid and gas phases are also too complicated to let Fick's law/species A concentration gradient account for the mass transfer alone.

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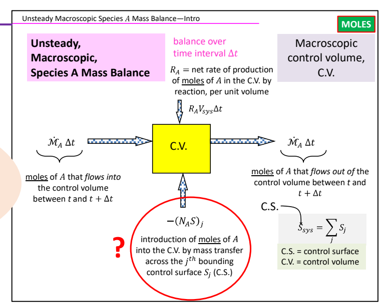
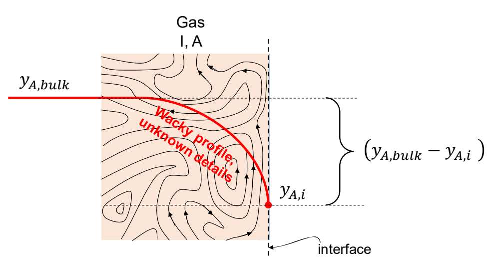
Linear Driving Force Model for Mass Transfer

Linear Driving Force (LDF) Model for Mass Transfer





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

Bulk convection present—Linear-driving-force model

Consider a <u>less</u> <u>idealized</u> situation:

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

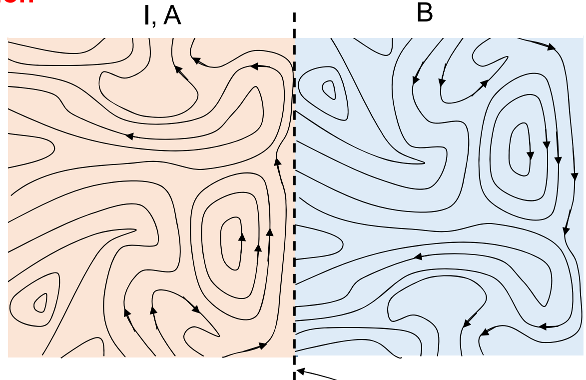
e.g. gas absorption

Both fluids are **in motion**

Gas I, A

Liquid B

$y_{A,bulk}$



$x_{A,bulk}$

Bulk flow is present.

interface

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

?

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Bulk convection present—Linear-driving-force model

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

e.g. gas absorption

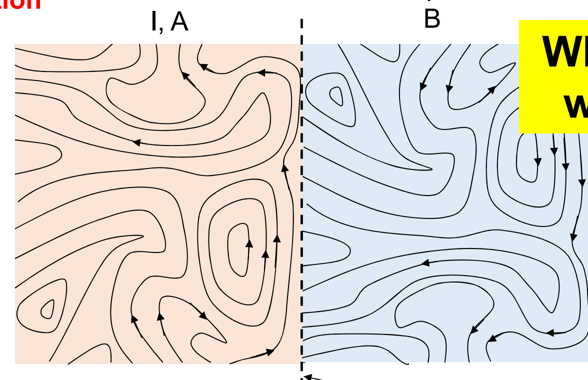
Both fluids are **in motion**

Gas I, A

Liquid B

What can we do?

$y_{A,bulk}$



$x_{A,bulk}$

Bulk flow is present.

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

?

WRF, Ch29 p 596

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Bulk convection present—Linear-driving-force model

Heat Transfer review

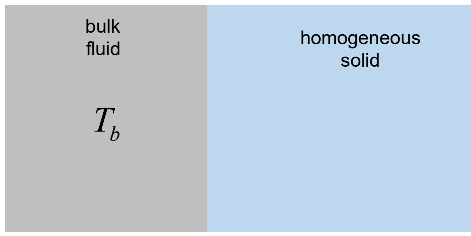
Remember *Newton's law of cooling*?

What about this case?

CM3110

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

Heat Transfer review

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CM3110

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What is the flux at the wall?

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Bulk convection present—Linear-driving-force model

Heat Transfer review

Remember *Newton's law of cooling*?

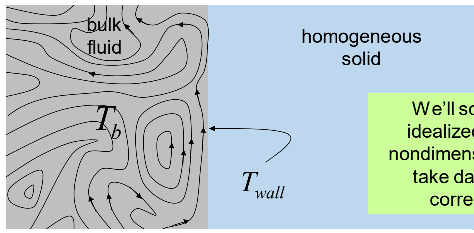
This was a case of heat transfer to an interface (a fluid-solid interface).

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!

$$T_b \neq T_{wall}$$

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

What is the flux at the wall?

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Bulk convection present—Linear-driving-force model

Heat Transfer review

Remember *Newton's law of cooling*?

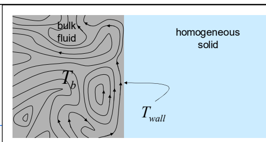
= **linear-driving-force model**

Newton's law of cooling assumes the heat flux is **proportional to the heat-transfer driving force, ΔT_{df}**

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

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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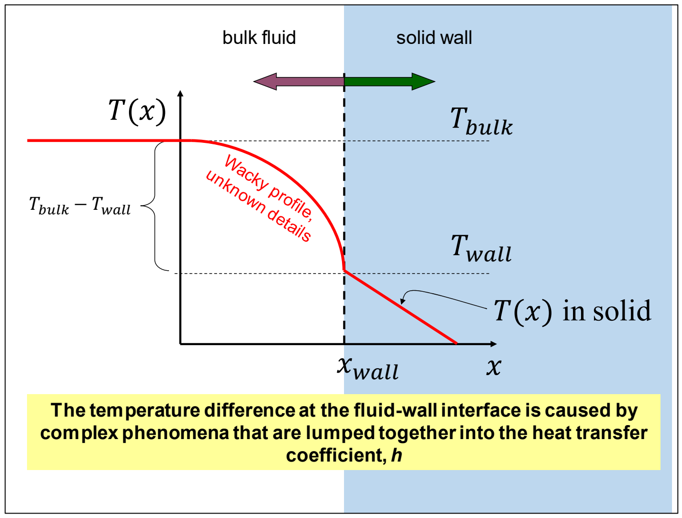
Bulk convection present—Linear-driving-force model

Heat Transfer review

Remember *Newton's law of cooling*?

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



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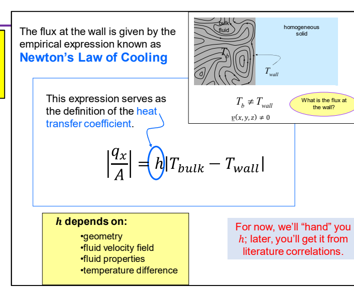
Bulk convection present—Linear-driving-force model

Heat Transfer review

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
- $1/h$ 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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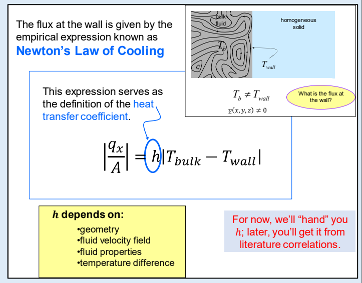
Bulk convection present—Linear-driving-force model

Inspiration:

We now do the same with mass transfer coefficient:

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



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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- This identifies the appropriate dimensionless numbers
- We take data and correlate using the dimensionless numbers
- $1/h$ 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.

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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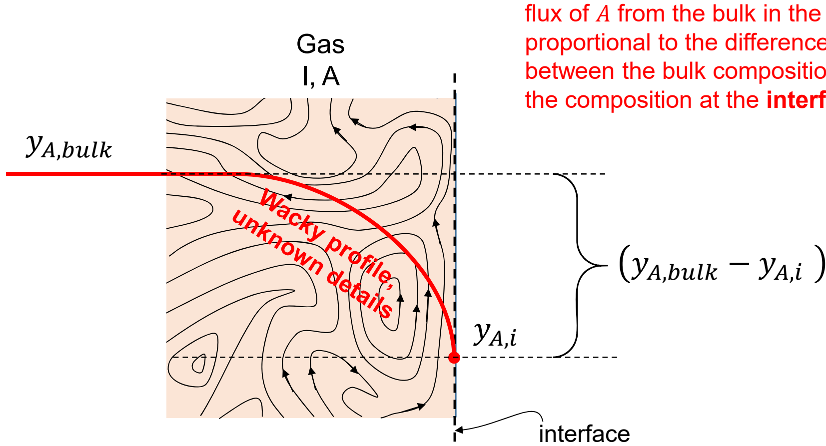
Bulk convection present—Linear-driving-force model

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

The driving-force : is a composition difference between the bulk the **interface**.

These "film coefficients" are based on mass transfer to the *interface*

WRF, Ch29 p 596

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Bulk convection present- Linear-driving-force model

There are numerous concentration units in use (practical consideration)

Linear-driving-force model (film coefficients): 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 film mass-transfer coefficients:

Table 29.1 Individual mass-transfer coefficients

Driving force	Flux equation	Units of k
Gas film		
Partial pressure (p_A)	$N_A = k_G(p_A - p_{A,i})$	kgmole/m^2 · s · atm
Concentration (c_A)	$N_A = k_c(c_{AG} - c_{AG,i})$	kgmole/(m^2 · s · (kgmole/m^3)) or m/s
Mole fraction (y_A)	$N_A = k_y(y_A - y_{A,i})$	kgmole/m^2 · s
Liquid film		
Concentration (c_{AL})	$N_A = k_L(c_{AL,i} - c_{AL})$	kgmole/(m^2 · s · (kgmole/m^3)) or m/s
Mole fraction (x_A)	$N_A = k_x(x_{A,i} - x_A)$	kgmole/m^2 · s

WRF, Ch29 p 596

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Overall Mass-Transfer Coefficient

concentrated regime

Liquid-phase-units:
Film Linear driving force model:

$$N_A \equiv k_x(x_{A,i} - x_{A,b})$$
$$N_A \equiv k_{cL}(c_{AL,i} - c_{AL,b})$$

Gas-phase-units:
Film Linear driving force model:

$$N_A \equiv k_p(p_{A,b} - p_{A,i})$$
$$N_A \equiv k_{cG}(c_{AG,b} - c_{A,i})$$
$$N_A \equiv k_y(y_{A,b} - y_{A,i})$$

Let's take these tools out for a spin!

Liquid-phase-units
Overall Linear driving force model:

$$N_A \equiv K_x(x_A^*(\ ) - x_{A,b})$$
$$N_A \equiv K_{cL}(c_{AL}^*(\ ) - c_{AL,b})$$

$(\ ) = p_{A,b}\ or\ c_{A,b}\ or\ y_{A,b}$

Gas-phase-units:
Overall Linear driving force model:

$$N_A \equiv K_p\left(p_{A,b} - p_A^*(\ )\right)$$
$$N_A \equiv K_{cG}\left(c_{AG,b} - c_{AG}^*(\ )\right)$$
$$N_A \equiv K_y\left(y_{A,b} - y_A^*(\ )\right)$$

$(\ ) = x_{A,b}\ or\ c_{AL,b}$

Warning: There's even more complexity coming

$$K_x = \frac{1}{\frac{1}{k_x} + \frac{1}{m'' k_y}},\quad K_y = \frac{1}{\frac{1}{k_y} + \frac{m'}{k_x}},\ \text{etc.}$$

Bulk convection present—Linear-driving-force model

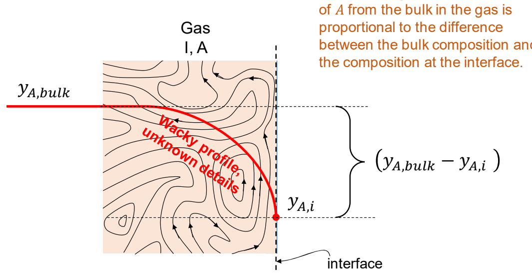
With this method, we do not model the details of the diffusion and convection in the gas.

Instead, we propose that the net effect is that flux is proportional to the mass-transfer **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

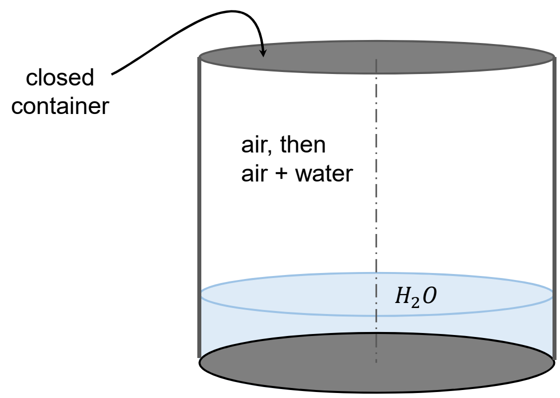
$$N_A = k_y(y_{A,bulk} - y_{A,i})$$

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

WRF, Ch29 p 596

Unsteady Macroscopic Species A Mass Balance

Example 7: Bone dry air and liquid water (water volume $= 0.80\ liters$) are introduced into a closed container (cross sectional area $= 150\ cm^2$; total volume $= 19.2\ liters$). Both air and water are at 25^oC, $\sim 1.0\ atm$ throughout this scenario. Three minutes after the air and water are placed in the closed container, the vapor is found to be 5.0% saturated with water vapor. What is the mass transfer coefficient for the water transferring from the liquid to the gas? How long will it take for the gas to become 90% saturated with water?



Cussler, p239, FAM v54 p59

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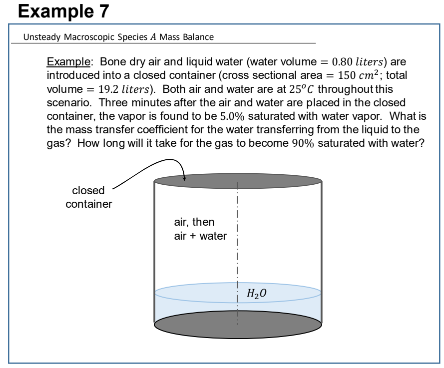
Unsteady Macroscopic Species A Mass Balance

What is our model?

(our assumptions)

1. Control volume =
2.

Example 7


Unsteady Macroscopic Species A Mass Balance

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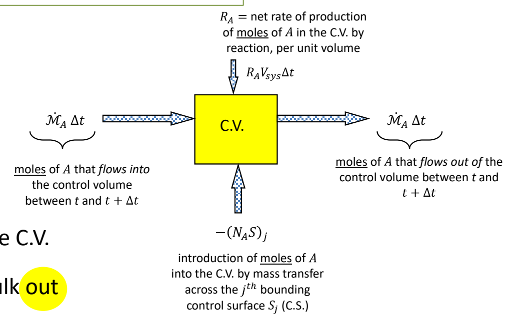
Unsteady Macroscopic Species A Mass Balance

MOLES

accumulation = net flow in + production + introduction

$$\frac{d}{dt}\left(\mathcal{M}_{A,sys}\right) = -\Delta\dot{\mathcal{M}}_A + R_A V_{sys} - \sum_j (N_A S)_j$$



$\mathcal{M}_{A,sys} = c_A V_{sys}$ = total moles of A in the C.V.

$\Delta\dot{\mathcal{M}}_A = \sum_{j,outs} \dot{\mathcal{M}}_{A,j} - \sum_{j,ins} \dot{\mathcal{M}}_{A,j}$ = bulk out

R_A = net rate of production of moles of A in the C.V. by reaction, per unit volume

V_{sys} = system volume

$N_{A_j} = K\Delta c_{df}$ =molar flux of A out through the j^{th} C.S.

$S_{sys} = \sum_j S_j$
Δ is "out"- "in"
C.S. = control surface
C.V. = control volume

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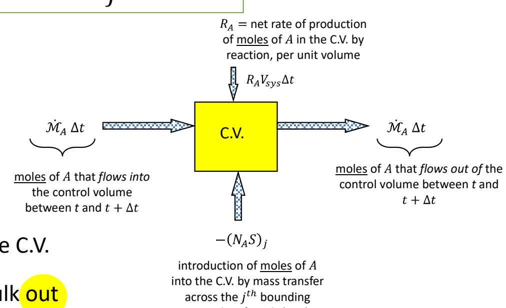
Unsteady Macroscopic Species A Mass Balance

MOLES

accumulation = net flow in + production + introduction

$$\frac{d}{dt}\left(\mathcal{M}_{A,sys}\right) = -\Delta\dot{\mathcal{M}}_A + R_A V_{sys} - \sum_j (N_A S)_j$$

The choice of the "system," i.e. of the *control volume,* is an important first step.



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(think "source" and "sink")

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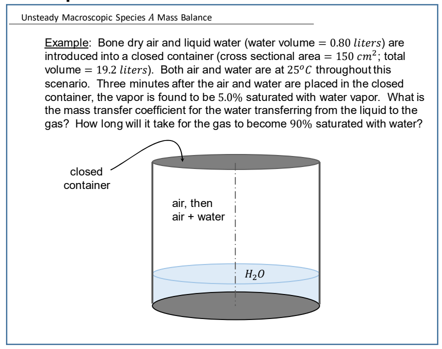
Example 7



Unsteady Macroscopic Species A Mass Balance

Example: Bone dry air and liquid water (water volume $= 0.80\ liters$) are introduced into a closed container (cross sectional area $= 150\ cm^2$; total volume $= 19.2\ liters$). Both air and water are at 25^oC throughout this scenario. Three minutes after the air and water are placed in the closed container, the vapor is found to be 5.0% saturated with water vapor. What is the mass transfer coefficient for the water transferring from the liquid to the gas? How long will it take for the gas to become 90% saturated with water?

Solution:

(mass transfer coefficient for evaporating water)

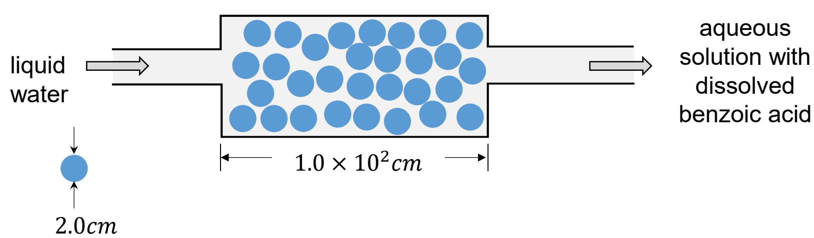
$$k_c = 3.4 \times 10^{-2} cm/s$$

$$\frac{c_A}{c_A^*} = 1 - e^{-\left(\frac{k_c S}{V_{gas}}\right)t}$$

$$t = 2.3\ hours$$

Homework 4.13

Example 8: Flow through a packed bed of soluble spherical pellets.



Two-centimeter diameter spheres of benzoic acid (soluble in water) are packed into a bed as shown. The spheres have $23\ cm^2$ of surface area per cm^3 volume of bed. What is the mass transfer coefficient when pure water flowing in ("superficial velocity"= $5.0\ cm/s$) exits 62% saturated with benzoic acid?

Cussler, p240, FAM v54 p63

Unsteady Macroscopic Species A Mass Balance

What is our model?

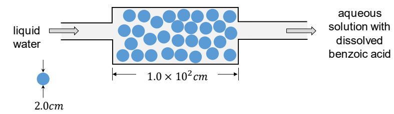
(our assumptions)

1. Control volume =
2.

Example 8

Unsteady Macroscopic Species A Mass Balance

Example: Flow through a packed bed of soluble spherical pellets.



Two centimeter diameter spheres of benzoic acid (soluble in water) are packed into a bed as shown. The spheres have $23\ cm^2$ of surface area per cm^3 volume of bed. What is the mass transfer coefficient when pure water flowing in ("superficial velocity"= $5.0\ cm/s$) exits 62% saturated with benzoic acid?

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Unsteady Macroscopic Species A Mass Balance

Solution:

(dissolving benzoic acid in packed bed, pseudo steady state)

$$k_c = \frac{v^0}{aL}\left(-\ln\left(1 - \frac{c_{AL}}{c_A^*}\right)\right)$$

$$k_c = 2.1 \times 10^{-3} cm/s$$

Example 8

Unsteady Macroscopic Species A Mass Balance

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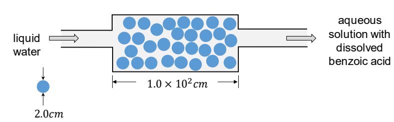

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Homework 4.12

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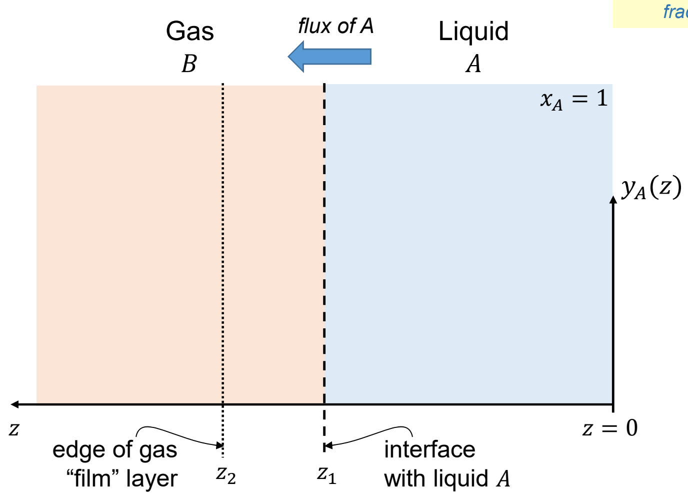
Bulk convection present—Linear-driving-force model

Example 9: 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

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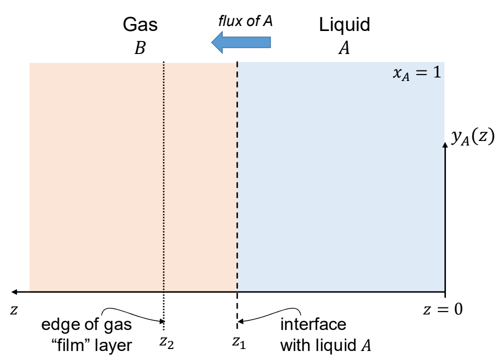

You try.

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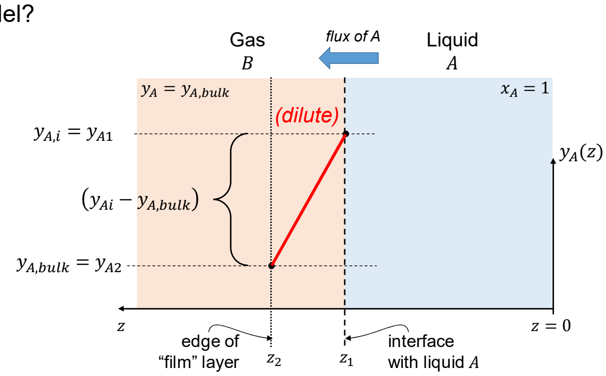

Solution:

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

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

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

Film model prediction for mass-transfer coefficient

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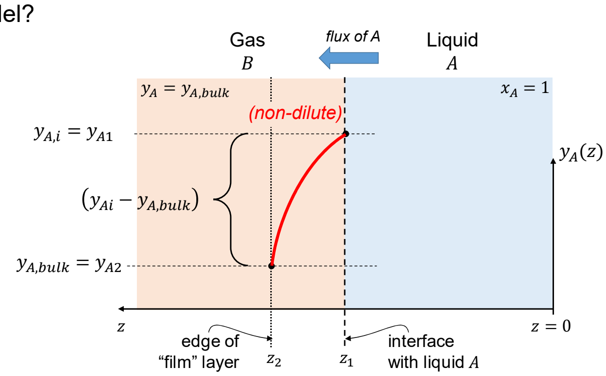

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Film model prediction for mass-transfer coefficient

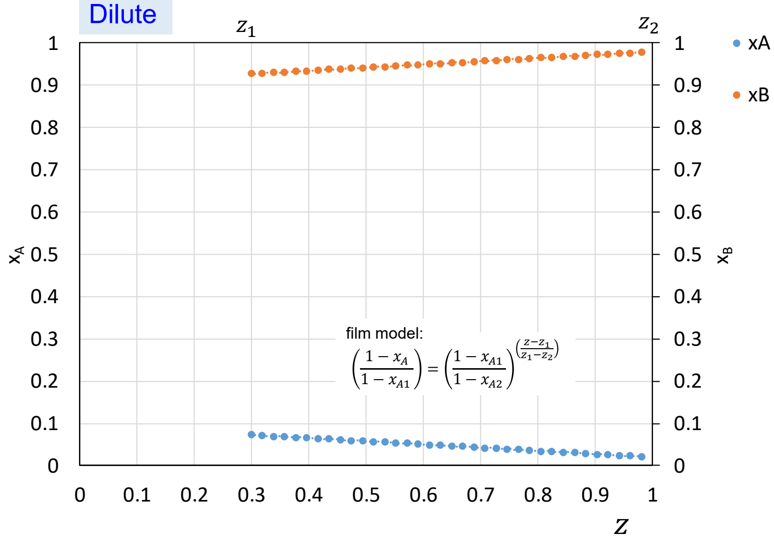
Bulk convection present—Linear-driving-force model

(see Example 1)

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

Dilute

DILUTE DILUTE DILUTE



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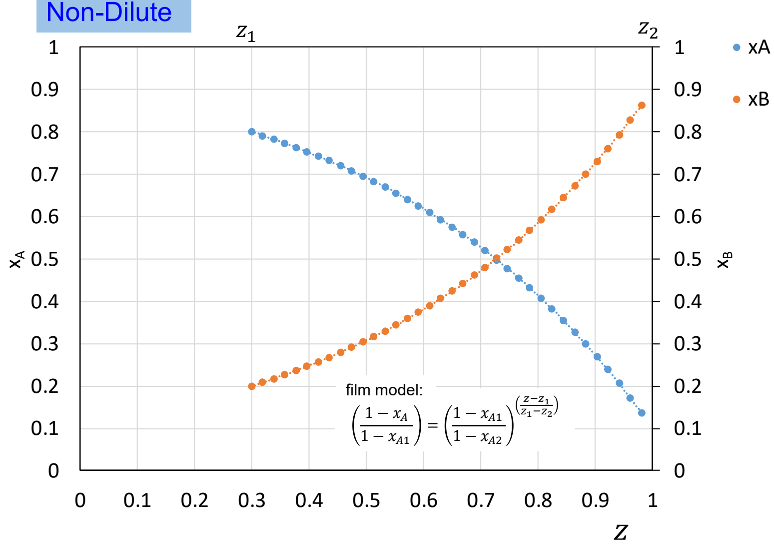
Bulk convection present—Linear-driving-force model

(Example 9)

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

Non-Dilute

NOT DILUTE



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Bulk convection present—Linear-driving-force model

Mass-transfer coefficient for film model

We used mole fraction units:

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

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

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

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

…

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

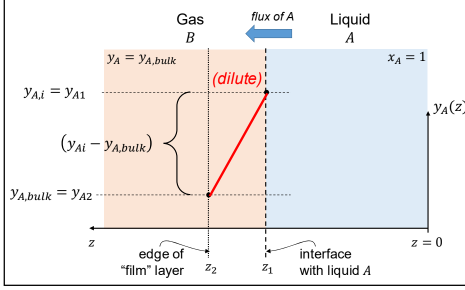
Film model prediction for mass transfer coefficient

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?



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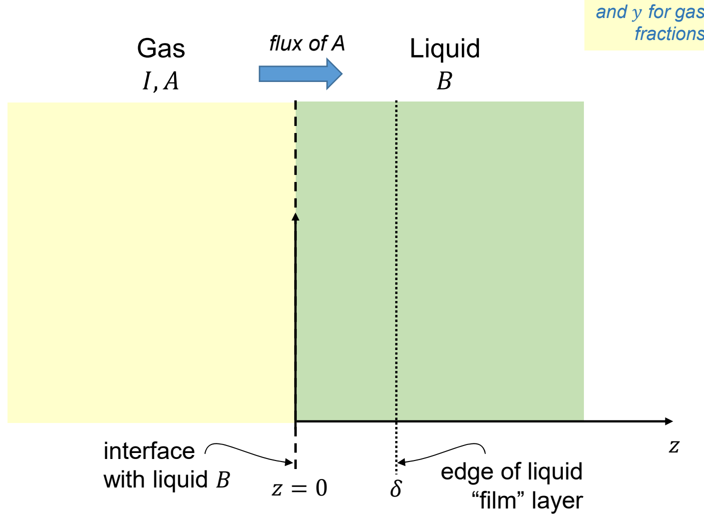
Bulk convection present—Linear-driving-force model

Example 10: 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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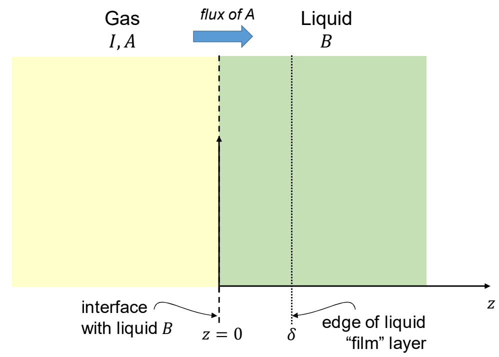
Bulk convection present—Linear-driving-force model

Example 10: 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.

Bulk convection present—Linear-driving-force model

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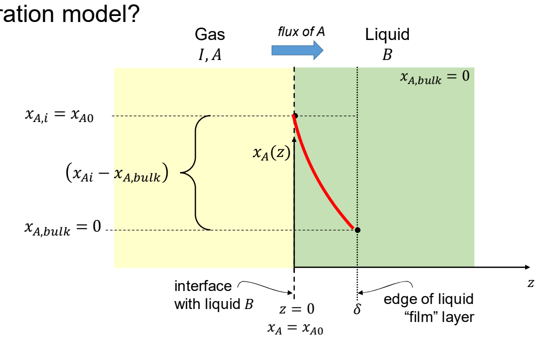


Solution:

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

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

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

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

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

Predicting Mass Transfer Coefficients

Mass transfer coefficient is an alternative to the diffusion coefficient as a way to quantify mass transfer.

- *Diffusion coefficient* is a material property
- *Mass transfer coefficient* is a scenario property

We can assess the accuracy of models (for a system) by measuring the dependence of k_c on $\mathcal{D}_{AB}$.

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	$k_c = 0.664\frac{D_{AB}}{L}Re_L^{1/2}Sc^{1/3}$	$k_c \propto D_{AB}^{2/3}$

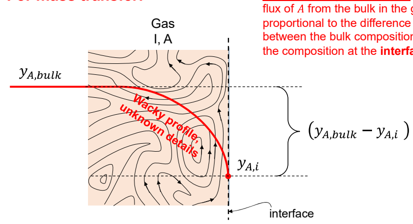
Mass transfer to an interface

Summary

- Flux to the interface = mass transfer coefficient × concentration-difference driving force
- Various units are in use
- Readily incorporated into macroscopic balances
- Film coefficients k_x, k_y, k_c determined experimentally
- $\mathcal{D}_{AB}$ models can be evaluated through k_x measurements

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

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

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

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

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