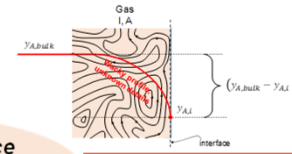
Contining work with the linear driving force for mass transfer, i.e. mass transfer coefficients, k_c

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

Mass Transport "Laws"

We 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 *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) $\mathrm{Sh} = f(\mathrm{ReSc})$
5. Facilitate combining resistances into overall mass transfer coefficients, K_L, K_G, to be used in modeling unit operations

Model macroscopic processes, design units

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)

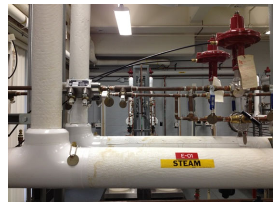
Linear-Driving-Force Model $|N_A| = k_y|y_{A,bulk} - y_{A,i}|$

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)

Overall Mass Transfer Coefficients

Michigan Tech

CM3110
Transport II
Part II: Diffusion and Mass Transfer



Overall Mass Transfer Coefficients

5

Professor Faith A. Morrison

Department of Chemical Engineering
Michigan Technological University

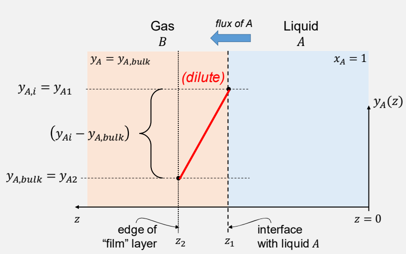
3

Modeling Mass Transfer Equipment—Overall Mass-Transfer Coefficient

Modeling Mass Transfer Equipment with the Overall Mass-Transfer Coefficient

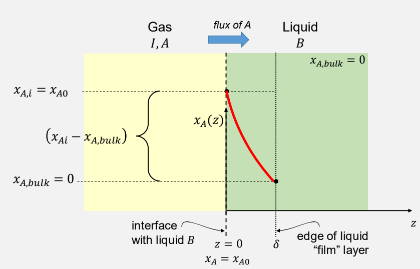
We have concerned ourselves with mass transfer to and from the ***bulk*** region of a phase and the ***interface*** with another phase:

From interface with liquid to bulk gas



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

From interface with gas, to bulk liquid



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

(lectures 9-10)

4

Modeling Mass Transfer Equipment—Overall Mass-Transfer Coefficient

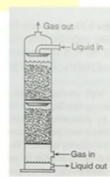
Modeling Mass Transfer Equipment with the
Overall Mass-Transfer Coefficient

We have also considered how to model mass transfer in ***chemical engineering process units***, such as ***gas absorbers***:

Gas Absorption

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

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



Begin lecture 8
Cussler, p305, 7

Let's review

(lectures 7-8)

5

REVIEW: Lectures 7-8—
1D Steady Diffusion Applied to Gas Absorption:

REVIEW REVIEW REVIEW REVIEW

Gas Absorption

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

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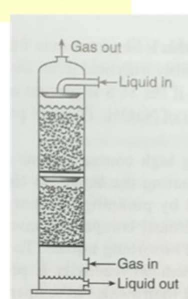


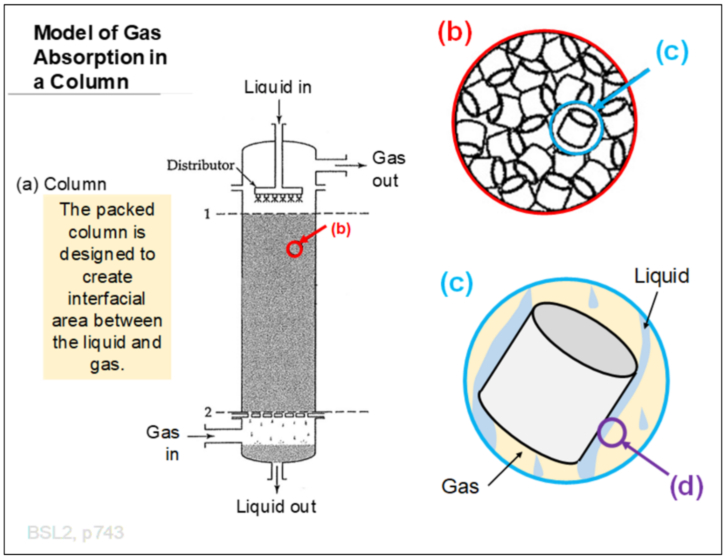
Begin lecture 8
Cussler, p305, 7

(lectures 7-8)

6

REVIEW: Lectures 7-8—
1D Steady Diffusion Applied to Gas Absorption:

REVIEW REVIEW REVIEW REVIEW



(lectures 7-8)

7

REVIEW: Lectures 7-8—
1D Steady Diffusion Applied to Gas Absorption:

REVIEW REVIEW REVIEW REVIEW

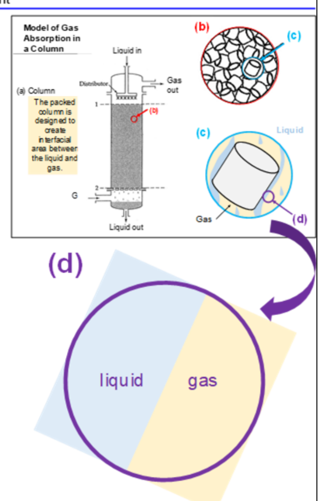
1D Steady Diffusion—Gas Absorption with Chemical Solvent

The Mass-Transfer Model

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

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

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

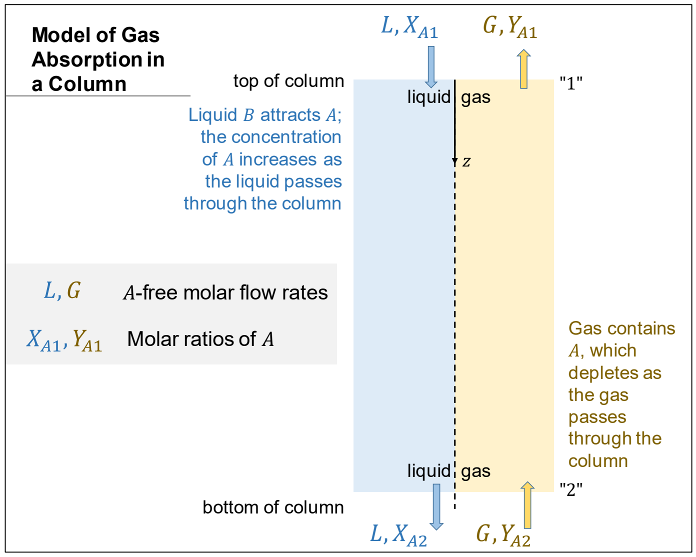


(lectures 7-8)

8

REVIEW: Lectures 7-8—
1D Steady Diffusion Applied to Gas Absorption:

REVIEW REVIEW REVIEW REVIEW

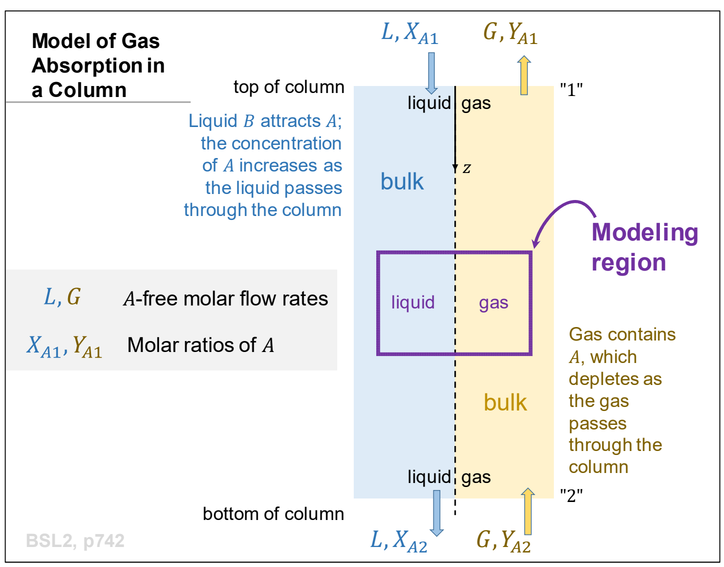


(lectures 7-8)

9

REVIEW: Lectures 7-8—
1D Steady Diffusion Applied to Gas Absorption:

REVIEW REVIEW REVIEW REVIEW



(lectures 7-8)

10

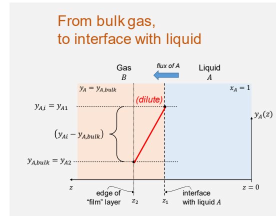
Modeling Mass Transfer Equipment—Overall Mass-Transfer Coefficient

Modeling Mass Transfer Equipment with the Overall Mass-Transfer Coefficient

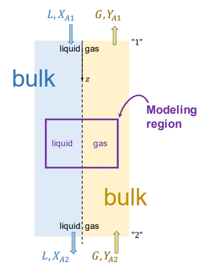
We have concerned ourselves with mass transfer to and from the ***bulk*** region of a phase and the ***interface*** with another phase

We have also considered how to model mass transfer in ***chemical engineering process units***, such as ***gas absorbers***

From bulk gas, to interface with liquid



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



We seek a *combined* model that allows us to describe mass transfer to/from ***bulk*** gas and ***bulk*** liquid.

This will help us to design and optimize chemical engineering mass-transfer units.

Our solution is inspired by how **heat exchangers** are modeled with overall heat transfer coefficient, ***U*** ...

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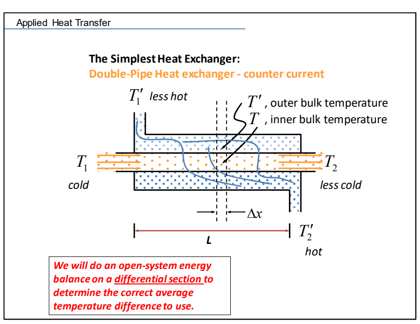
Modeling Mass Transfer Equipment—Overall Mass-Transfer Coefficient

Modeling Mass Transfer Equipment with the Overall Mass-Transfer Coefficient

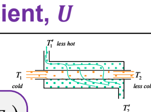
Heat exchangers are modeled with overall heat transfer coefficient, ***U***:

$$Q = UA\Delta T_{lm}$$



Overall heat transfer coefficient, *U*

Analysis of double-pipe heat exchanger



FINAL RESULT:

$$Q = U\underbrace{(2\pi RL)}_{A}\underbrace{\frac{(T_1' - T_1) - (T_2' - T_2)}{\ln\frac{(T_1' - T_1)}{(T_2' - T_2)}}}_{\equiv \Delta T_{lm}}$$

$$Q = UA\Delta T_{lm}$$

=log-mean temperature difference

ΔT_{lm} is the correct average temperature to use for the overall heat-transfer coefficients in a double-pipe heat exchanger.

We develop **overall mass transfer coefficients**, K_L, K_G

(lectures 7-8)

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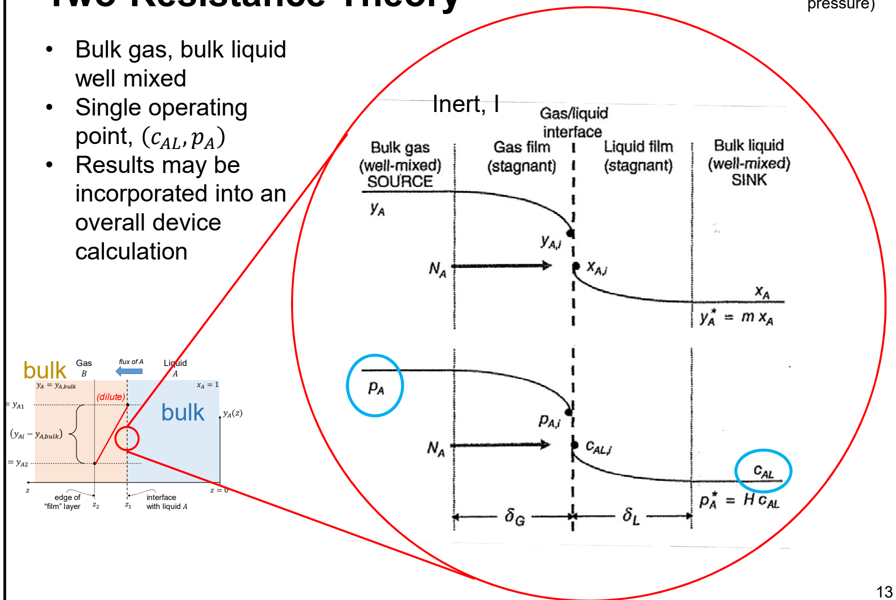
Modeling Mass Transfer Equipment—Overall Mass-Transfer Coefficient

(two sets of units shown, mole fractions, concentration/ pressure)

Two-Resistance Theory

- Bulk gas, bulk liquid well mixed
- Single operating point, (c_{AL}, p_A)
- Results may be incorporated into an overall device calculation



(lectures 7-8)

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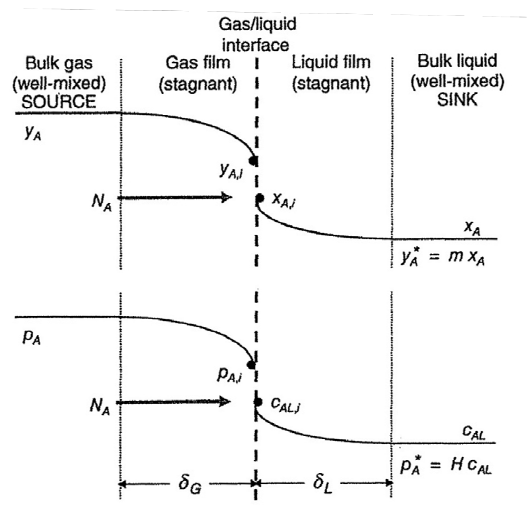
Modeling Mass Transfer Equipment—Overall Mass-Transfer Coefficient

Two-Resistance Theory

Bulk gas, bulk liquid well mixed



Liquid **equilibrium** characterized by m, the equilibrium distribution coefficient:

$$y_A = m x_A$$

Gas **equilibrium** characterized by H, the Henry's law constant:

$$p_A = H c_{AL}$$

WRF Ch29, Fig 29.4

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Mass-Transfer Coefficient—Two-Resistance Theory

For mass transfer, use the linear driving force model

Gas: Linear driving force model:

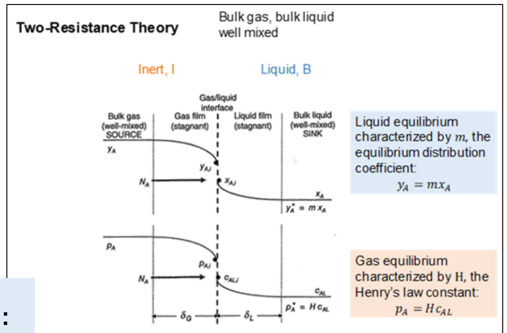
$$(N_A)_G = k_G(p_A - p_{Ai})$$

$$k_G[=]\frac{(moles\ A\ transferred)}{(time \cdot area \cdot pressure)}$$

Liquid: Linear driving force model:

$$(N_A)_L = k_L(c_{AL,i} - c_{AL})$$

$$k_L[=]\frac{(moles\ A\ transferred)}{(time \cdot area \cdot conc)}$$



$$(N_A)_G = (N_A)_L$$

WRF Ch29, Fig 29.4

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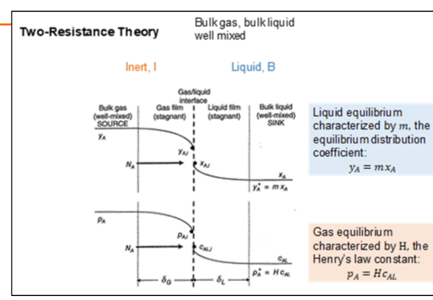
Mass-Transfer Coefficient—Two-Resistance Theory



Using the linear driving force model for mass transfer

$$(N_A)_G = (N_A)_L$$

$$k_G(p_A - p_{Ai}) = k_L(c_{AL,i} - c_{AL})$$

$$(p_A - p_{Ai}) = \frac{-k_L}{k_G}(c_{AL} - c_{AL,i})$$

(c_{AL}, p_A) = operating point

(c_{ALi}, p_{Ai}) = inteface point

We need to combine with the equilibrium relationship

WRF Ch29, Fig 29.4

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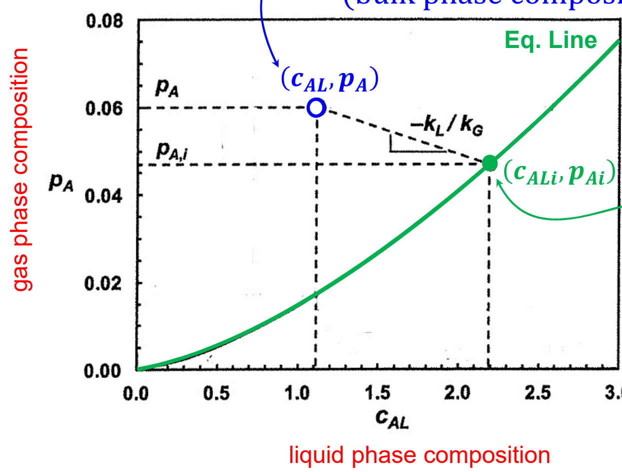
Mass-Transfer Coefficient—Two-Resistance Theory

Mass transfer: $(p_A - p_{Ai}) = \frac{-k_L}{k_G}(c_{AL} - c_{AL,i})$

(c_{AL}, p_A) = operating point (bulk phase compositions)



(c_{ALi}, p_{Ai}) = interface point (interface phase compositions; in equilibrium)

If k_G, k_L known from data correlations (dimensional analysis, literature), the operating point and the interface point may be linked.

WRF Ch29, Fig 29.6

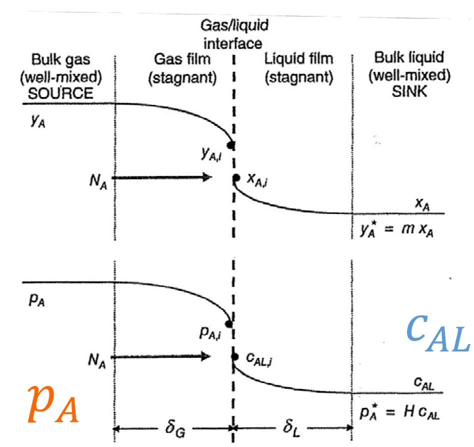
17

Mass-Transfer Coefficient—Two-Resistance Theory

Ideally, we could relate the two bulk phases directly:

$$N_A \overset{?}{=} K(p_A - c_{AL})$$

Inert, I Liquid, B



WRF Ch29

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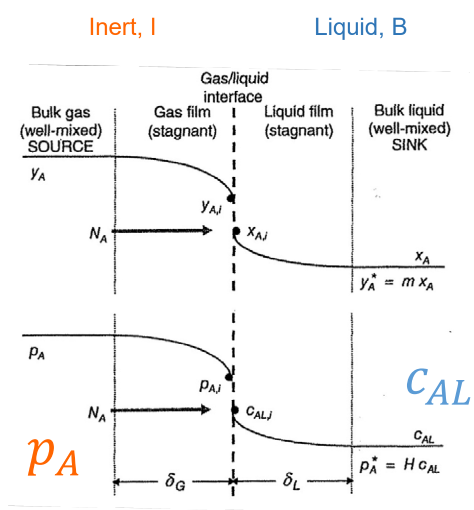
Mass-Transfer Coefficient—Two-Resistance Theory

Ideally, we could relate the two bulk phases directly:

$$N_A \overset{?}{=} K(p_A - c_{AL})$$

But the units don't work!

?



WRF Ch29

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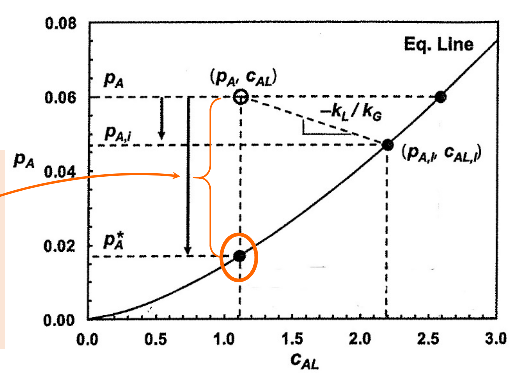
Mass-Transfer Coefficient—Two-Resistance Theory

Ideally, we could relate the two bulk phases directly:

$$N_A \overset{?}{=} K(p_A - c_{AL})$$

Gas:
<u>Overall</u> Linear driving force model:

$$N_A = K_G(p_A - p_A^*)$$



As a representation of the liquid phase composition, use the saturation pressure associated with liquid operating point concentration c_{AL}

(lectures 7-8)

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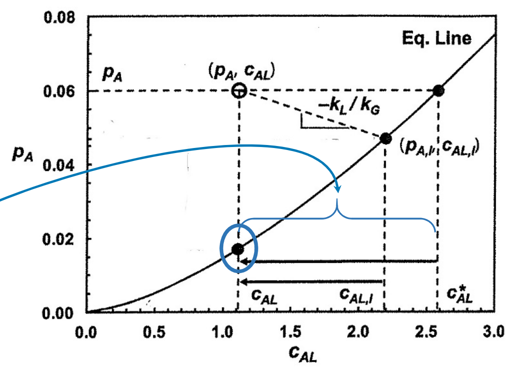
Mass-Transfer Coefficient—Two-Resistance Theory

Ideally, we could relate the two bulk phases directly:

$$N_A \overset{?}{=} K(p_A - c_{AL})$$

Liquid
<u>Overall</u> Linear driving force model:

$$N_A = K_L(c_{AL}^* - c_{AL})$$



As a representation of the gas phase composition use the saturation concentration associated with gas phase operating point pressure p_A

(lectures 7-8)

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Mass-Transfer Coefficient—Two-Resistance Theory

Ideally, we could relate the two bulk phases directly:

$$N_A \overset{?}{=} K(p_A - c_{AL})$$

Liquid
<u>Overall</u> Linear driving force model:

$$N_A = K_L(c_{AL}^* - c_{AL})$$

Gas:
<u>Overall</u> Linear driving force model:

$$N_A = K_G(p_A - p_A^*)$$

Overall Mass Transfer Coefficients

Two versions; one based on gas phase customary units, one based on liquid phase customary units

How can we interrelate these?

(lectures 7-8)

22

Mass-Transfer Coefficient—Two-Resistance Theory

How can we interrelate these?

Liquid
Overall Linear driving force model:

$$N_A = K_L(c_{AL}^* - c_{AL})$$

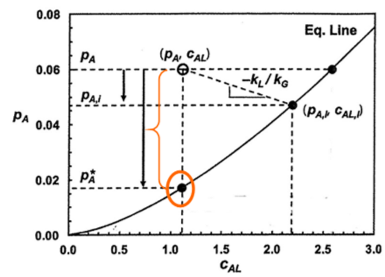
Gas:
Overall Linear driving force model:

$$N_A = K_G(p_A - p_A^*)$$

$$N_A = K_G(p_A - p_A^*)$$

Assuming linear equilibrium relationship (not shown) for liquid operating point c_{AL}:

$$p_A^* = Hc_{AL}$$



(lectures 7-8)

23

Mass-Transfer Coefficient—Two-Resistance Theory

Overall Mass Transfer Coefficients

Liquid
Overall Linear driving force model:

$$N_A = K_L(c_{AL}^* - c_{AL})$$

Gas:
Overall Linear driving force model:

$$N_A = K_G(p_A - p_A^*)$$

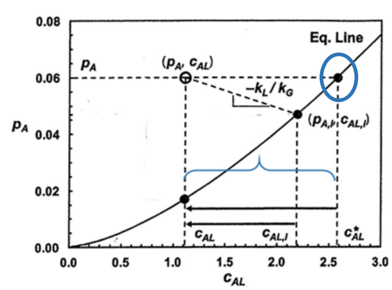
$$N_A = K_G(p_A - p_A^*)$$

Assuming linear equilibrium relationship (not shown) for liquid operating point c_{AL}:

$$p_A^* = Hc_{AL}$$

And assuming linear equilibrium for gas operating point p_A:

$$p_A = Hc_{AL}^*$$



We can relate the overall mass transfer coefficients K_G, K_L with those based on mole factions…

(lectures 7-8)

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Mass-Transfer Coefficient—Two-Resistance Theory

Overall Mass Transfer Coefficients

Liquid
Overall Linear driving force model:

$$N_A = K_L(c_{AL}^* - c_{AL})$$

Gas:
Overall Linear driving force model:

$$N_A = K_G(p_A - p_A^*)$$

We can relate the overall mass transfer coefficients K_G, K_L with individual mass transfer coefficients and those based on mole fractions…

$$\frac{1}{K_G} = \frac{(p_A - p_A^*)}{N_A} = \frac{p_A - p_{Ai}}{N_A} + \frac{p_{Ai} - p_A^*}{N_A}$$

$$\frac{1}{K_G} = \frac{p_A - p_{Ai}}{N_A} + \frac{H(c_{ALi} - c_{AL})}{N_A}$$

$$\frac{1}{K_G} = \frac{1}{k_G} + \frac{H}{k_L}$$

$$\frac{1}{K_y} = \frac{1}{k_y} + \frac{m}{k_x}$$

Note: limited to linear equilibrium curve (see text for nonlinear)

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Mass-Transfer Coefficient—Two-Resistance Theory

Overall Mass Transfer Coefficients

Liquid
Overall Linear driving force model:

$$N_A = K_L(c_{AL}^* - c_{AL})$$

Gas:
Overall Linear driving force model:

$$N_A = K_G(p_A - p_A^*)$$

We can relate the overall mass transfer coefficients K_G, K_L with individual mass transfer coefficients and those based on mole fractions…

$$\frac{1}{K_L} = \frac{(c_{AL}^* - c_{AL})}{N_A} = \frac{c_{AL} - c_{ALi}}{N_A} + \frac{c_{ALi} - c_{AL}}{N_A}$$

$$\frac{1}{K_L} = \frac{p_A - p_{Ai}}{HN_A} + \frac{(c_{ALi} - c_{AL})}{N_A}$$

$$\frac{1}{K_L} = \frac{1}{Hk_G} + \frac{1}{k_L}$$

$$\frac{1}{K_x} = \frac{1}{mk_y} + \frac{1}{k_x}$$

Note: limited to linear equilibrium curve (see text for nonlinear)

26

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:

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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Mass-Transfer Coefficient—Two-Resistance Theory

Overall Mass Transfer Coefficients

Liquid
Overall Linear driving force model:

$$N_A = K_L(c_{AL}^* - c_{AL})$$

Gas:
Overall Linear driving force model:

$$N_A = K_G(p_A - p_A^*)$$

Example:
WRF Example 1 page 604 (solution in text)

A liquid stripping process ($20^oC, 1.5\ atm$) is used to transfer hydrogen sulfide (H_2S) dissolved in water into an air stream. At the present conditions of operations the composition of H_2S in the bulk phase is $1.0\ mole\%$ and in the liquid phase is $0.0006\ mole\%$. The individual mass-transfer coefficients are $k_x = 0.30\ kmol/m^2s$ for the liquid film and $k_y = 4.5 \times 10^{-3} mol/m^2s$ for the gas film. Calculate the flux, the overall mass transfer coefficients, and the interface composition.

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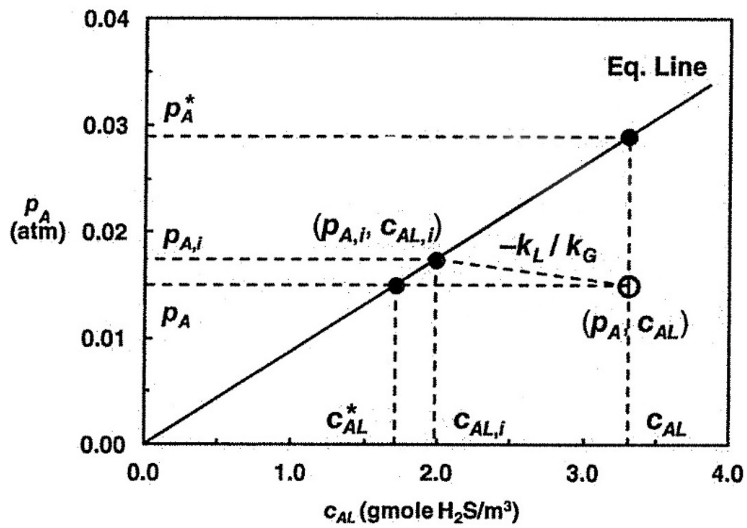
Example:
WRF Example 1 page 604 (solution in text)



WRF p604, Fig 29.8

Overall Mass Transfer Coefficients

Summary

- Specific to a device (not a material, not a detailed model of interphase mass transfer)
- Allow the overall driving force to be quantified (within its assumptions)
- May be used in design of units
- The approach for the overall design is to apply the transfer at an arbitrary location z and integrate over the entire column
- Individual mass transfer coefficients are needed to determine the overall transfer coefficients (obtain from literature)

Liquid
Overall Linear driving force model:

$$N_A = K_L(c_{AL}^* - c_{AL})$$

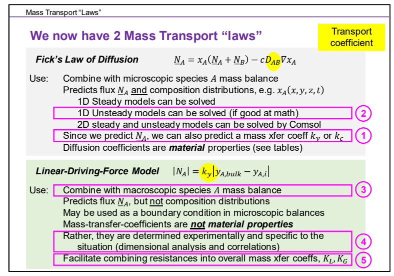
Gas:
Overall Linear driving force model:

$$N_A = K_G(p_A - p_A^*)$$

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 *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 *Model macroscopic processes, design units*
4. ✓ Are not material properties; rather, they are determined experimentally and specific to the situation (dimensional analysis and correlations) $\mathrm{Sh} = f(\mathrm{ReSc})$
5. ✓ Facilitate combining resistances into overall mass transfer coefficients, K_L, K_G, to be used in modeling unit operations *Combine resistances to mass transfer in a process unit into an overall resistance*

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As teachers we can choose between

(a) sentencing students to thoughtless mechanical operations and
(b) facilitating their ability to think.

If students' readiness for more involved thought processes is bypassed in favor of jamming more facts and figures into their heads, they will stagnate at the lower levels of thinking. But if students are encouraged to try a variety of thought processes in classes, they this can … develop considerable mental power. Writing is one of the most effective ways to develop thinking.

—Syrene Forsman

Reference: Forsman, S. (1985). "Writing to Learn Means Learning to Think." In A. R. Gere (Ed.), *Roots in the sawdust: Writing to learn across the disciplines* (pp. 162-174). Urbana, IL: National Council of Teachers of English.

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