See also Krishna & Wesselingh Chem. Eng. Sci. 52(6) 1997 861-911

Mass transfer and separation technology

Massöverföring och separationsteknik ("MÖF-ST")

Appendix. Mass transfer in multi-component mixtures

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A.1 "Old-school" mass transfer

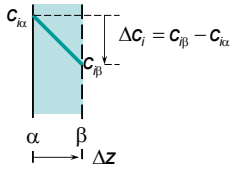
Mass Transfer as you have learned it

J_i : flux of *i* with respect to the mixture

$$J_i = -D\frac{dc_i}{dz}$$ **Fick's law**

$$J_i = -D_i\frac{\Delta c_i}{\Delta z} = -k_i \Delta c_i \qquad k_i = \frac{D_i}{\Delta z}$$

diffusivity *mass transfer coefficient*



Diffusion with Drift

N_i : flux with respect to an interface

flux of mixture $N = \sum_i N_i$

differential equation $N_i = -D_i\frac{dc_i}{dz} + Nx_i$

difference equation $N_i = \underbrace{-k_i \Delta c_i}_{\text{diffusion flux}} + \underbrace{N\bar{x}_i}_{\text{drift flux}} \longrightarrow -k_i s_i \Delta c_i$

Stefan or drift correction

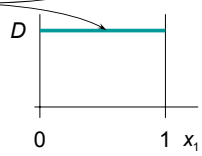
Classic - in Gases

gas: $c_1 + c_2 = c = constant$

fluxes with respect to mixture

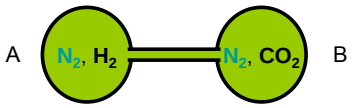
$$J_1 = -D_1\frac{dc_1}{dz}$$
$$J_2 = -D_2\frac{dc_2}{dz}$$
$$+$$
$$J_1 + J_2 = 0 = -D\frac{d(c_1 + c_2)}{dz}$$

only one binary *D*, which is independent of composition



Three Gases (1)

ideal gases, 100 kPa, 298 K

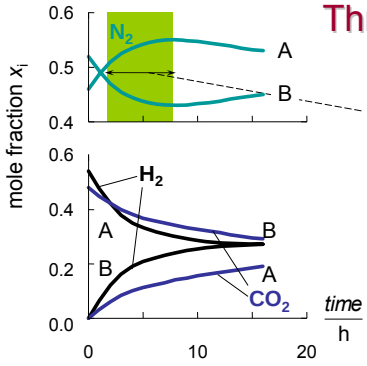


beginning: $x_{N2} = 0.46$ $x_{H2} = 0.54$ | $x_{N2} = 0.52$ $x_{CO2} = 0.48$

Question: Does N_2 transfer
(a) from A to B? (b) from B to A?
(c) not at all? (d) or does it do (a), (b) and (c)?

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Three Gases (2)

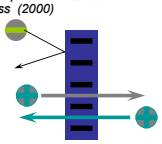


reverse diffusion

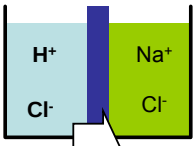
Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Two Cations

cation permeable membrane



high concentration



low concentration

(1) *H^+ moves rapidly* so Na^+ can move **against** its concentration gradient!

(2) → *excess +charge and electrical field*

(3)

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

2 Gases in a Porous Plug (1)

He 298 K 100 kPa | Ar 298 K 100 kPa

$$N_{He} \approx -3 N_{Ar} \quad !$$

$$\sqrt{\frac{M_{Ar}}{M_{He}}}$$

friction (He / **plug**) < friction (Ar / **plug**)

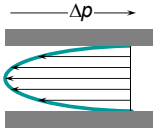
→ *the plug, matrix or membrane is a (pseudo)component*

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

2 Gases in a Porous Plug (2)

He 298 K 100 kPa | Ar 298 K **101** kPa *(for example)*

$$N_{He} = -N_{Ar}$$



main reason: **viscous flow**

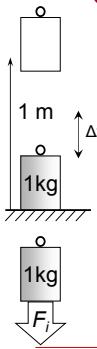
retards He, *accelerates* Ar

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

A.2 Driving forces

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Gravity - a simple Potential



- the potential difference is the work required to change the condition of the weight

  here: $\Delta\psi = mg\,\Delta z = 9.81\ \text{J} \quad (\equiv 9.81\ \text{Nm})$

  or, per mole $\Delta\psi_i = M_i g\,\Delta z$

- the driving force is the negative potential gradient: $F_i = -\frac{d\psi_i}{dz} = -M_i g$

  the force is downwards

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Chemical Potential

x_i γ_i mixture

chemical potential

$$\mu_i = const(p,T) + RT\ln a_i$$

$$a_i = \gamma_i x_i$$

activity *activity coefficient*

work required: change in the chemical potential

pure *i* (one mole)

$$\mu_i^* = const(p,T)$$

$$\Delta\mu_i = \mu_i^* - \mu_i = -RT\ln a_i$$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

μ in an Ideal Solution

chemical potential in an ideal solution $\mu_i = const\,(p,T) + RT \ln x_i$

in an ideal gas $\mu_i = const(p,T) + RT \ln\left(\frac{p_i}{p}\right)$

partial pressure

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Momentum Balance

forces $\sum F$

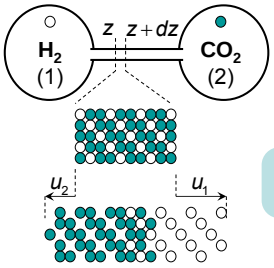
momentum 'in' $\sum(\dot{m}v)_{in}$

momentum 'out' $\sum(\dot{m}v)_{out}$

change of momentum $\frac{d(mv)}{dt} = \sum(\dot{m}v)_{in} - \sum(\dot{m}v)_{out} + \sum F$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Moving Through Each Other

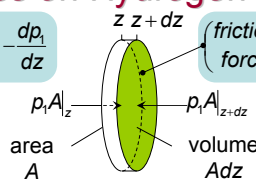


species velocities

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Forces on Hydrogen (1)

$\left(\text{driving force}\right) = -\frac{dp_1}{dz}$



$\left(\text{friction force}\right) \propto p_1 p_2 (u_2 - u_1)$

Force balance: $-\frac{dp_1}{dz} \propto p_1 p_2 (u_1 - u_2)$ force per volume

with $c_1 = \frac{p_1}{RT}$ gives $-\frac{RT}{p_1}\frac{dp_1}{dz} \propto RT p_2 (u_1 - u_2)$ force per mole

Driving force $F_1 \propto RT p_2 (u_1 - u_2) = \zeta_{1,2} x_2 (u_1 - u_2)$

with friction coefficient $\zeta_{1,2} = \frac{RT}{D_{1,2}} = \frac{RT}{D_{2,1}} = \zeta_{2,1}$

Note: often $x_2 \approx 1$ and $u_2 = 0$

Gases: $u \sim 10^{-2}$ m/s
Liquids: $u \sim 10^{-4}$ m/s

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Driving Force (per Mole of *i*)

$$F_i = -\frac{d\mu_i}{dz} = -RT\frac{d\ln a_i}{dz} = -\frac{RT}{a_i}\frac{da_i}{dz} \rightarrow -\frac{RT}{x_i}\frac{dx_i}{dz}$$

for a given T and p *in ideal solutions*

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Maxwell-Stefan Equation

$$F_i = \sum_{j \neq i} \zeta_{i,j} x_j (u_i - u_j)$$

driving force on *i*

friction coefficient between *i* and *j*

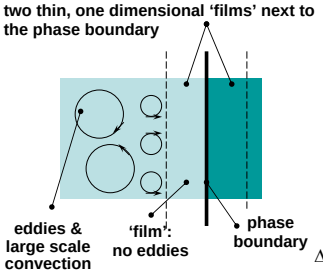
mole fraction of *j*

(diffusive) species velocities

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Film Theory, Thickness of Films

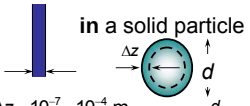
two thin, one dimensional 'films' next to the phase boundary



gases $\Delta z \approx 10^{-4}$ m

liquids $\Delta z \approx 10^{-5}$ m

in a solid particle



$\Delta z = 10^{-7} \ldots 10^{-4}$ m

$\Delta z \approx \frac{d}{10}$

membrane

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Difference Form of Force

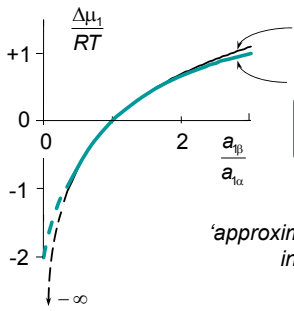
$$F_i = -\frac{\Delta \mu_i}{\Delta z} = -RT \frac{\Delta \ln a_i}{\Delta z} = -\frac{RT}{\bar{a}_i} \frac{\Delta a_i}{\Delta z} \rightarrow -\frac{RT}{\bar{x}_i} \frac{\Delta x_i}{\Delta z}$$

for a given T and p

in ideal solutions

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Approximation



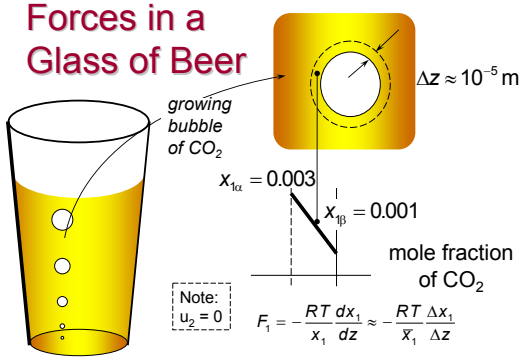
exact $\ln\left(\frac{a_{i\beta}}{a_{i\alpha}}\right)$

approximate $\frac{\Delta a_1}{\bar{a}_1} = \frac{a_{i\beta} - a_{i\alpha}}{0.5(a_{i\beta} + a_{i\alpha})}$

'approximate' works out better in difference equations

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Forces in a Glass of Beer



$$F_1 = -\frac{RT}{x_1} \frac{dx_1}{dz} \approx -\frac{RT}{\bar{x}_1} \frac{\Delta x_1}{\Delta z}$$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Example (3.1 from book)

3.1 A species in a gas has a molar mass of $M = 0.03$ kg mol^{-1}. The gas diffuses through a film with a thickness $\Delta z = 10^{-4}$ m. The velocity of the gas changes from $u_\alpha = 1$ cm s^{-1} to $u_\beta = 2$ cm s^{-1}. There are driving forces and friction forces on the species. The driving force during transport through a film has a value of 10^7 N mol^{-1}. The momentum balance for the species reads:

$$F_{omi}^{driving} + F_{omi}^{friction} = \frac{\Delta(M_i u_i)}{\Delta t}$$

How does the change in momentum compare with the driving force?

Example (3.1 from book): answer

3.1 The residence time in the film is $\bar{u} = 1.5\times10^{-2}\ ms^{-1} \rightarrow\ \Delta t = \Delta z/u = 7\times10^{-3}$ s resulting in a change in the momentum:

$$\Delta(M_i u_i) \quad (3\times10^{-2})\times(1\times10^{-2})\,\text{kg mol}^{-1}\,\text{m s}^{-1} \qquad \sim1\times10^{-2}\,\text{N mol}^{-1}$$

This is negligible compared to the driving force.

A.3 Friction

Friction Coefficients of Spheres

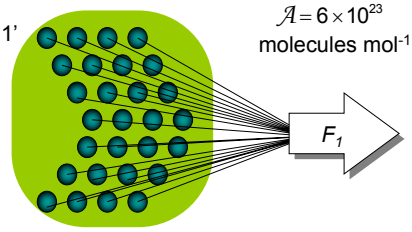
coefficient of a single sphere

$$\zeta_{1,2} = \mathcal{A}\times\overbrace{3\pi\eta_2 d_1} \approx 3\times10^{12}\ \text{N mol}^{-1}\left(\text{m s}^{-1}\right)^{-1}$$

$\mathcal{A} = 6\times10^{23}$ molecules mol^{-1}

spheres '1'

liquid '2'



See PTG § 6.7: Stokes Law

Diffusion and Friction Coefficients

$$Đ_{1,2} \equiv \frac{RT}{\zeta_{1,2}} \qquad \zeta_{1,2} \equiv \frac{RT}{Đ_{1,2}}$$

- each others 'inverse'
- we use both

$$Đ_{1,2} = \frac{RT}{\mathcal{A}3\pi\eta_2 d_1} \rightarrow \frac{8.314\times300}{6\times10^{23}\times10\times10^{-3}\times\left(0.4\times10^{-9}\right)} \approx 10^{-9}\frac{\text{m}^2}{\text{s}}$$

Maxwell-Stefan diffusivity of large molecules in dilute liquids (*not* gases)

One Equation Missing

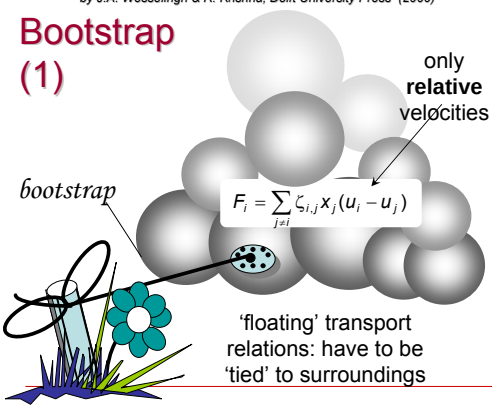
- 2 components: 1 relative velocity → 1 independent equation
- 3 components: 2 relative velocities → 2 independent equations
- *n* components: *n* - 1 relative velocities → *n* - 1 independent equations

Bootstrap (1)

only **relative** velocities

bootstrap

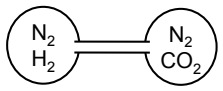
$$F_i = \sum_{j\neq i}\zeta_{i,j}x_j(u_i - u_j)$$



'floating' transport relations: have to be 'tied' to surroundings

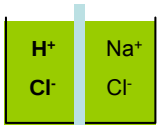
Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Bootstraps (2)



- no net volume flow

- plug does not move



- membrane does not move
- (almost) no charge transfer

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Fluxes

- in practical problems we use **fluxes**:

$$N_i = \bar{u}_i \bar{c}_i = \bar{u}_i \bar{c} \bar{x}_i$$

- flux form of MS-equation:

$$F_i c x_i = \sum_j \zeta_{i,j} c x_i x_j (u_i - u_j)$$

F_i / V ; $x_i = c_i / c$

$$\rightarrow \quad f_i = \sum_j \zeta_{i,j} (x_j N_i - x_i N_j)$$

force on *i* per unit volume of mixture

Multi-component mass transfer
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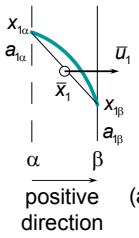
From Differential to Difference



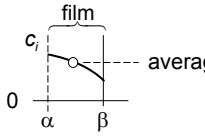
binary:
$$-\frac{RT}{a_1}\frac{da_1}{dz} = x_2 \frac{RT}{Đ_{1,2}}(u_1 - u_2)$$

infinitesimal layer
$$-\frac{da_1}{a_1} = x_2 \frac{(u_1 - u_2)}{(Đ_{1,2}/dz)}$$

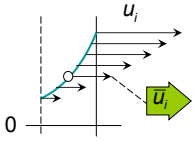
finite layer (approximate)
$$-\frac{\Delta a_1}{\bar{a}_1} = \bar{x}_2 \frac{(\bar{u}_1 - \bar{u}_2)}{k_{1,2}} \qquad k_{1,2} = \frac{Đ_{1,2}}{\Delta z}$$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Average Velocity



average concentration $\bar{c}_i$



species velocity (depends on position in film)

species velocity at the average composition

→ *positive velocity*

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Differences with Fluxes

$$-\frac{\Delta a_1}{\bar{a}_1} = \frac{1}{k_{1,2}} \bar{x}_2 (\bar{u}_1 - \bar{u}_2) \quad \times \frac{\bar{c}\bar{x}_1}{\bar{c}}$$

$$\rightarrow \quad -\bar{x}_1 \frac{\Delta a_1}{\bar{a}_1} = \frac{1}{k_{1,2}\bar{c}} (\bar{x}_2 N_1 - \bar{x}_1 N_2)$$

Multi-component mass transfer
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Multicomponent Equations

using velocities

$$-\frac{\Delta a_i}{\bar{a}_i} = \sum_{j \neq i} \bar{x}_j \frac{(\bar{u}_i - \bar{u}_j)}{k_{i,j}}$$

for ideal solutions

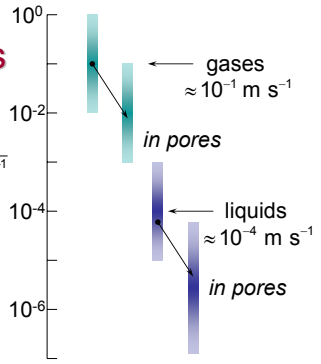
using fluxes

$$-\bar{x}_i \frac{\Delta a_i}{\bar{a}_i} = \sum_{j \neq i} \frac{(\bar{x}_j N_i - \bar{x}_i N_j)}{k_{i,j}\bar{c}}$$

$-\Delta x_i$

Transfer Coefficients

$k_{i,j} = \frac{Đ_{i,j}}{\Delta z}$ $\quad \frac{k_{i,j}}{\mathrm{m\,s^{-1}}}$



Temperature Effects

MS-equation

$$F_i = \sum_j \zeta_{i,j} x_j (u_i - u_j) + (\text{thermal diffusion terms})$$

small

driving force

$$F_i = -\left(\frac{d\mu_i}{dz}\right)_T = -\frac{RT}{x_i}\frac{dx_i}{dz}$$

at constant temperature

difference form:

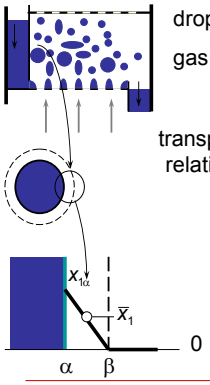
$$F_i = -\frac{R\bar{T}}{\bar{x}_i}\frac{\Delta x_i}{\Delta z}$$

average film temperature

changes are not very important

A.4 Binary examples

Stripping - dilute



drops on a tray

gas: trace of NH_3 (1)

bulk of N_2 (2)

transport relation

$$-\Delta x_1 = \frac{\bar{x}_2 N_1 - \bar{x}_1 N_2}{k_{1,2}\bar{c}}$$

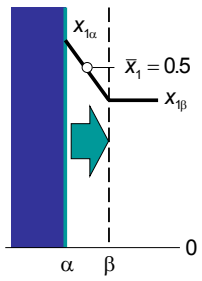
$\bar{x}_2 \approx 1 \quad N_2 = 0$

bootstrap

flux $\quad N_1 = -k_{1,2}\bar{c}\Delta x_1$

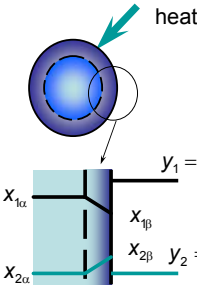
..as you already knew..

Stripping - concentrated



$$N_1 = -\frac{k_{1,2}\bar{c}}{\bar{x}_2}\Delta x_1 = (-2)\,k_{1,2}\bar{c}\Delta x_1$$

Vaporising Droplet



benzene (1), volatile

toluene (2)

vapour removed by convection

bootstrap: $\frac{N_1}{N_2} = \frac{y_1}{y_2} = \nu$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Fluxes from Vaporising Droplet

$$-\Delta x_1 = \frac{\bar{x}_2 N_1 - \bar{x}_1 N_2}{k_{1,2} c} \qquad -\Delta x_2 = \frac{\bar{x}_1 N_2 - \bar{x}_2 N_1}{k_{1,2} c}$$

$$\frac{N_1}{N_2} = \nu \qquad N_1 = -\frac{k_{1,2} c}{\bar{x}_2 - \bar{x}_1/\nu}\Delta x_1 \qquad N_2 = -\frac{k_{1,2} c}{\bar{x}_1 - \bar{x}_2 \nu}\Delta x_2$$

example $\nu = 2 \quad \bar{x}_1 = \bar{x}_2 = 0.5$

$$\longrightarrow \quad N_1 = -4 k_{1,2} c \Delta x_1 \qquad N_2 = -(-2) k_{1,2} c \Delta x_2$$

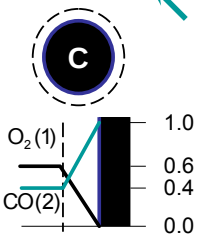
$\Delta x_1 < 0$
$\Delta x_2 > 0$

Stefan (drift) corrections

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Carbon Gasification

$O_2 + 2C \rightarrow 2CO$



both components are moving and have a high concentration

$k_{1,2} = 10^{-2}$ ms^{-1} $\quad c = 10$ mol m^{-3}

bootstrap:

$N_2 = -2N_1$

calculate N_1 and N_2

Multi-component mass transfer
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Fluxes in Gasification

$N_2 = -2N_1$

$$-\Delta x_1 = \frac{\bar{x}_2 N_1 - \bar{x}_1 N_2}{k_{1,2} c} = \frac{(\bar{x}_2 + 2\bar{x}_1) N_1}{k_{1,2} c}$$

$$N_1 = -\frac{k_{1,2} c}{\bar{x}_2 + 2\bar{x}_1}\Delta x_1 = -\frac{10^{-2} \times 10}{0.7 + 2 \times 0.3}(-0.6)$$

$N_1 = 0.046$ $(exact: 0.047)$ mol m^{-2} s^{-1}

$N_2 = -0.092$ $(exact :- 0.094)$ mol m^{-2} s^{-1}

almost the same

Multi-component mass transfer
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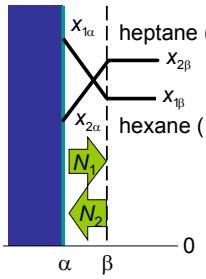
Binary Distillation



transport relation

$$-\Delta x_1 = \frac{\bar{x}_2 N_1 - \bar{x}_1 N_2}{k_{1,2} c}$$

bootstrap $N_1 = -N_2$

(equimolar exchange)

$$\rightarrow -\Delta x_1 = \frac{(\bar{x}_1 + \bar{x}_2) N_1}{k_{1,2} c}$$

$N_1 = -k_{1,2} c \Delta x_1 \qquad N_2 = -k_{1,2} c \Delta x_2$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Some Bootstraps

①	membrane stagnant	$u_M = 0$
②	bulk stagnant (absorption)	$N_2 = 0$
③	trace stagnant (polarisation)	$\bar{u}_1 = 0$
④	equimolar exchange (distillation)	$N_1 + N_2 = 0$
⑤	interface determined (vaporisation)	$\frac{N_1}{N_2} = \frac{y_1}{y_2}$
⑥	reaction stoichiometry	$\frac{N_1}{\nu_1} = \frac{N_2}{\nu_2}$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

A.5 Ternary examples

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Ternary - per mole of *i*

$$-\frac{d\mu_1}{dz} = \zeta_{1,2}x_2(u_1-u_2) + \zeta_{1,3}x_3(u_1-u_3)$$

forces per mole of '1'

$$-\frac{d\mu_2}{dz} = \zeta_{2,1}x_1(u_2-u_1) + \zeta_{2,3}x_3(u_2-u_3)$$

forces per mole of '2'

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Ternary - per mole of Mixture

$$-x_1\frac{d\mu_1}{dz} = \zeta_{1,2}x_1x_2(u_1-u_2) + \zeta_{1,3}x_1x_3(u_1-u_3)$$

$$-x_2\frac{d\mu_2}{dz} = \zeta_{2,1}x_1x_2(u_2-u_1) + \zeta_{2,3}x_2x_3(u_2-u_3)$$

forces per mole of mixture

these should cancel:

$\zeta_{2,1} \equiv \zeta_{1,2}$ $Đ_{2,1} \equiv Đ_{1,2}$ $k_{2,1} \equiv k_{1,2}$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

More Components

binary

$$-\Delta x_1 = \frac{\bar{x}_2N_1 - \bar{x}_1N_2}{k_{1,2}\bar{c}} + \frac{\bar{x}_3N_1 - \bar{x}_1N_3}{k_{1,3}\bar{c}}$$

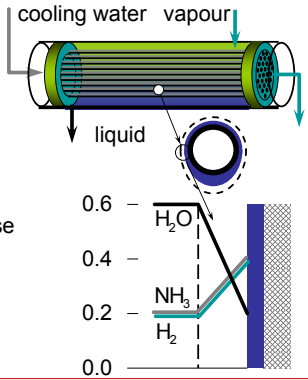
$$-\Delta x_2 = \frac{\bar{x}_1N_2 - \bar{x}_2N_1}{k_{2,1}\bar{c}} + \frac{\bar{x}_3N_2 - \bar{x}_2N_3}{k_{2,3}\bar{c}}$$

ternary

quaternary

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Condensor



Mix: NH_3+H_2O + H_2

NH_3 (1) and H_2O (2) condense on a tube

H_2 (3) does not condense

$k_{1,2} = 1\times10^{-3}$ ms^{-1}

$k_{1,3} = k_{2,3} = 3\times10^{-3}$ ms^{-1}

find the velocities in the gas film

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Condenser (2)

transport (MS) relations:

$$NH_3: \quad -0.2 = \frac{0.4N_1 - 0.3N_2}{(1\times10^{-3})30} + \frac{0.3N_1 - 0.4N_3}{(3\times10^{-3})30}$$

$$H_2O: \quad 0.4 = \frac{0.4N_2 - 0.3N_1}{(1\times10^{-3})30} + \frac{0.3N_2 - 0.3N_3}{(3\times10^{-3})30}$$

bootstrap $N_3 = 0$

three linear equations, three unknowns

$\longrightarrow$ $N_1 = 0.015$ $N_2 = 0.045$ mol m^{-2} s^{-1}

exact solutions: $N_1 = 0.013$ $N_2 = 0.049$ mol m^{-2} s^{-1}

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

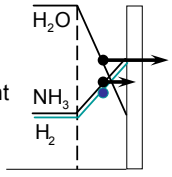
Condenser (3)

mixture velocity

H_2O moves *down* its gradient

NH_3 dragged *against* its gradient

H_2 does *not move at all*



Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Ternary Distillation (1)

① ethanol ③ water
② a trace of butanol

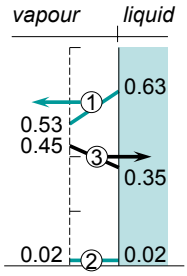
large friction between ① and ②

$k_{1,2} = 8 \times 10^{-2}$ ms^{-1}

$k_{1,3} = k_{2,3} = 20 \times 10^{-2}$ m s^{-1}

bootstrap: equimolar exchange

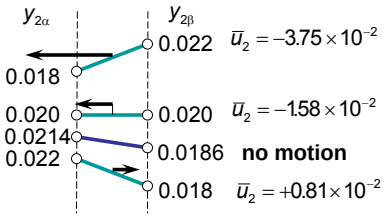
$\bar{u}_1 \bar{y}_1 + \bar{u}_2 \bar{y}_2 + \bar{u}_3 \bar{y}_3 = 0$



in which direction does ② move?

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

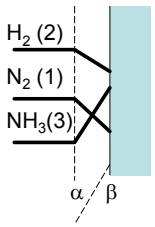
Butanol - which direction?



Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Ammonia reaction

$N_2 + 3H_2 \Leftrightarrow 2NH_3$



catalytic surface

transport relations:

$$-\Delta x_1 = \frac{\bar{x}_2 N_1 - \bar{x}_1 N_2}{k_{1,2} c} + \frac{\bar{x}_3 N_1 - \bar{x}_1 N_3}{k_{1,3} c}$$

$$-\Delta x_2 = \frac{\bar{x}_1 N_2 - \bar{x}_2 N_1}{k_{1,2} c} + \frac{\bar{x}_3 N_2 - \bar{x}_2 N_3}{k_{2,3} c}$$

$$-\Delta x_3 = \frac{\bar{x}_1 N_3 - \bar{x}_3 N_1}{k_{1,3} c} + \frac{\bar{x}_2 N_3 - \bar{x}_3 N_2}{k_{2,3} c}$$

bootstrap: $\frac{N_1}{1} = \frac{N_2}{3} = \frac{N_3}{-2}$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

When is: 3 = 2?

a **ternary** can be approximated as a **binary** when

$$-\frac{\Delta x_1}{\bar{x}_1} = \bar{x}_2 \frac{\bar{u}_1 - \bar{u}_2}{k_{1,2}} + \bar{x}_3 \frac{\bar{u}_1 - \bar{u}_3}{k_{1,3}} \quad \longrightarrow \quad \cdots = \bar{x}_{eff} \frac{\bar{u}_1 - \bar{u}_{eff}}{k_{1,eff}}$$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

① one friction term dominates:

$\frac{\bar{x}_2}{k_{1,2}} << \frac{\bar{x}_3}{k_{1,3}} \rightarrow \bar{x}_3 \frac{\bar{u}_1 - \bar{u}_3}{k_{1,3}}$ $\quad \bar{x}_{eff} = \bar{x}_3$ $\quad k_{1,eff} = k_{1,3}$

(example: mobile species in many membranes)

② equal velocity of two species:

$\bar{u}_2 = \bar{u}_3 \rightarrow \left(\frac{\bar{x}_2}{k_{1,2}} + \frac{\bar{x}_3}{k_{1,3}}\right)(\bar{u}_1 - \bar{u}_2)$ $\quad \frac{\bar{x}_{eff}}{k_{1,eff}} = \left(\frac{\bar{x}_2}{k_{1,2}} + \frac{\bar{x}_3}{k_{1,3}}\right)$

(example: Na^+ and Cl^- in water)

③ equal diffusivities *('1' in m- and p-xylene)* $\bar{x}_{eff} = \bar{x}_2 + \bar{x}_3$

$k_{1,2} = k_{1,3} \rightarrow \frac{(\bar{x}_2 + \bar{x}_3)\bar{u}_1 - (\bar{x}_2 \bar{u}_2 + \bar{x}_3 \bar{u}_3)}{k_{1,2}}$ $\quad \bar{u}_{eff} = \frac{\bar{x}_2 \bar{u}_2 + \bar{x}_3 \bar{u}_3}{\bar{x}_2 + \bar{x}_3}$

Multi-component mass transfer
using transparancies that accompany "Mass Transfer in Multicomponent mixtures" by J.A. Wesselingh & R. Krishna, Delft University Press (2000)

Effective Binary in Reactive System

simplifying transport equation of N_2 in ammonia formation:
eliminate N_2 and N_3 with $N_2 = 3N_1$ $\quad N_3 = -2N_1$

$\longrightarrow$ $N_1 = -k_{1,eff} c \Delta x_1$ with $\frac{1}{k_{1,eff}} = \frac{\bar{x}_2 - 3\bar{x}_1}{k_{1,2}} + \frac{\bar{x}_3 + 2\bar{x}_1}{k_{1,3}}$

similarly for H_2 and NH_3

If all fluxes Ni are related via the same reaction stoichiometry
→ pseudo - binary