TRANSPORT PHENOMENA II (0905342)

01- GLOBAL VIEW

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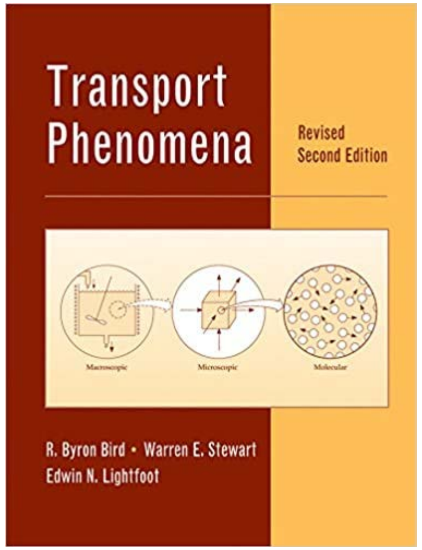
Outline

- Books
- Mass Transfer Mechanisms
- Kinds of Diffusion
- Importance of Mass Transfer
- Notation
- Fluxes
  - Convective
  - Molecular (Diffusive)
- Dimensionless Numbers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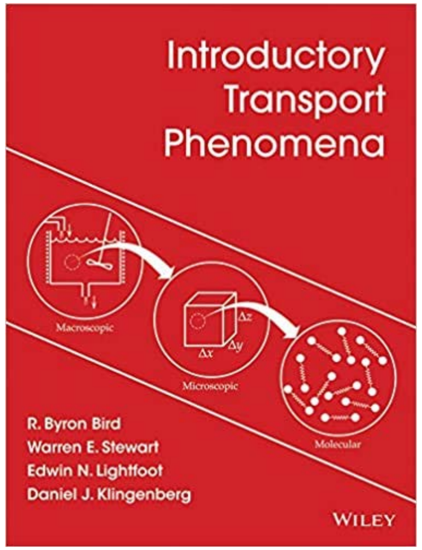
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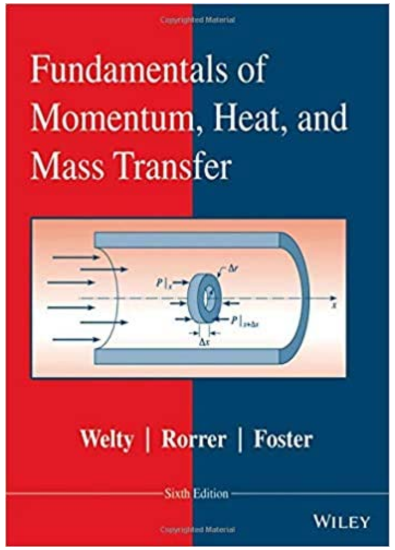
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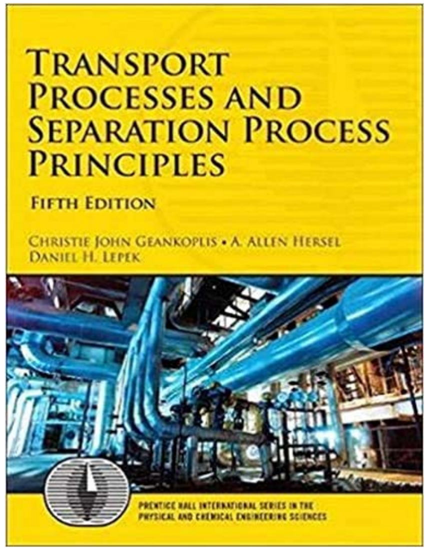
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PRINCIPLES
FIFTH EDITION
CHRISTIE JOHN GEANKOPLIS • A. ALLEN HERSEL
DANIEL H. LEPEK
PRENTICE HALL INTERNATIONAL SERIES IN THE
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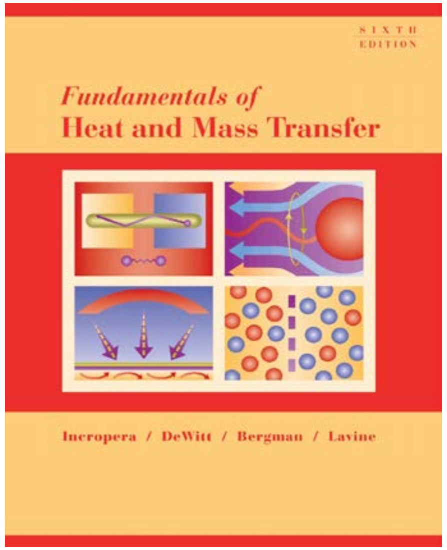
SIXTH
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Fundamentals of
Heat and Mass Transfer
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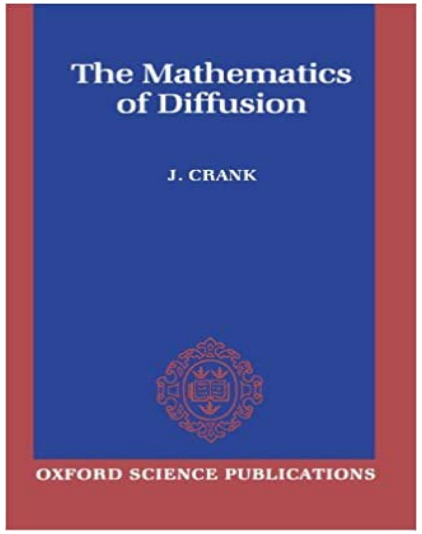
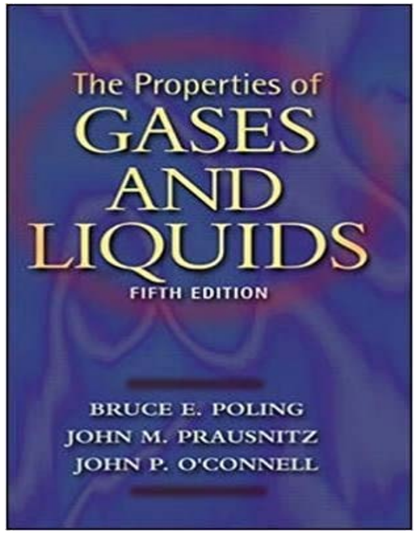

The Mathematics
of Diffusion
J. CRANK
OXFORD SCIENCE PUBLICATIONS


The Properties of
GASES
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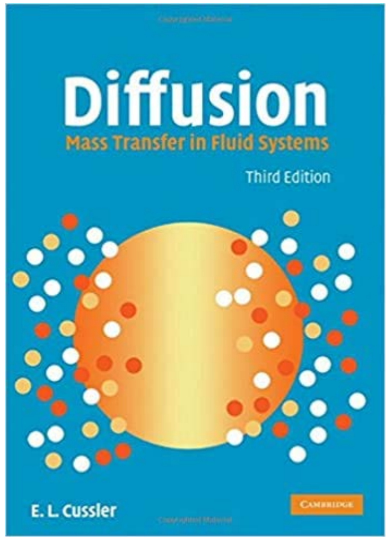
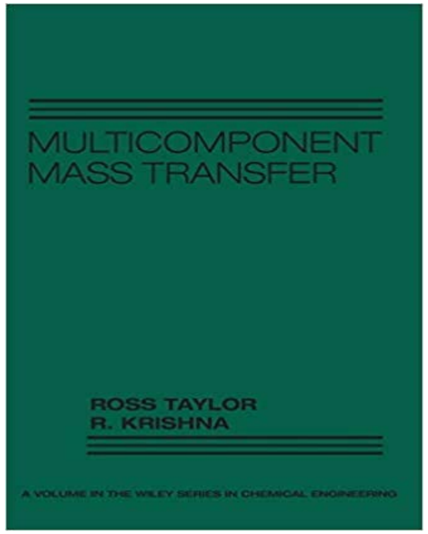
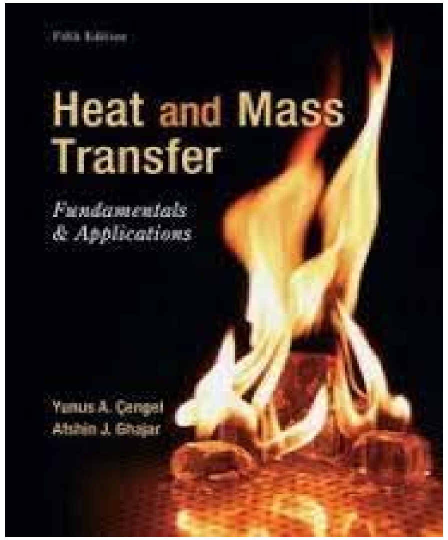
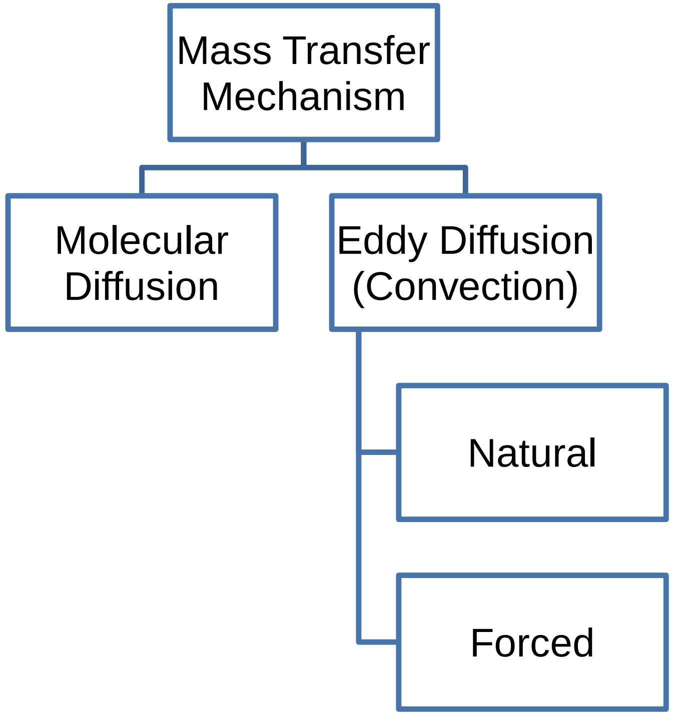
BRUCE E. POLING
JOHN M. PRAUSNITZ
JOHN P. O'CONNELL


Diffusion
Mass Transfer in Fluid Systems
Third Edition
E. L. Cussler
CAMBRIDGE


MULTICOMPONENT
MASS TRANSFER
ROSS TAYLOR
R. KRISHNA
A VOLUME IN THE WILEY SERIES IN CHEMICAL ENGINEERING


Heat and Mass
Transfer
Fundamentals
& Applications
Yunus A. Çengel
Afshin J. Ghajar

Mass Transfer Mechanisms



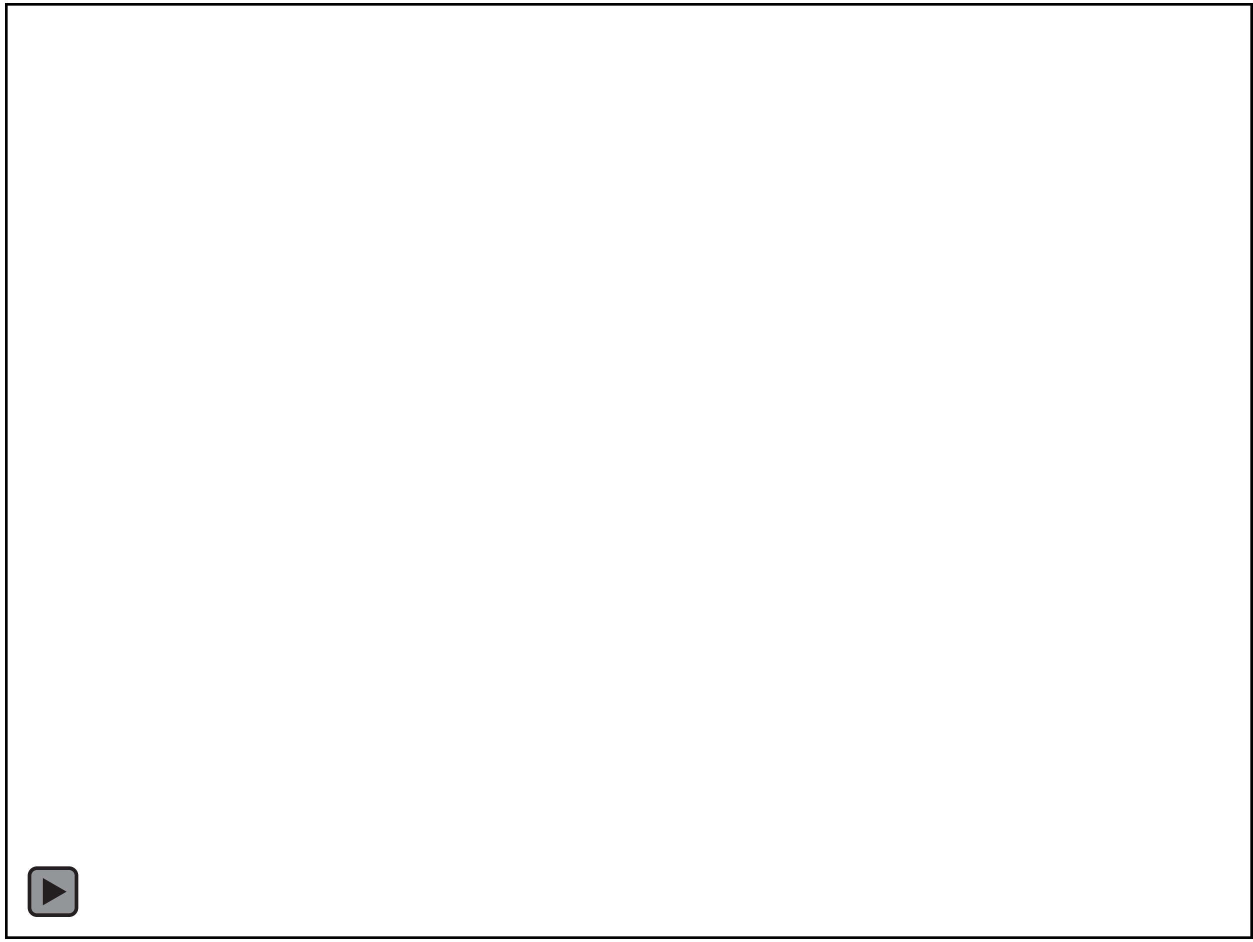
Molecular transport is always present in mass transfer. The fluxes always contain a molecular term plus a convective term

Mass transfer can occur within the same phase in a fluid mixture or across a phase boundary.

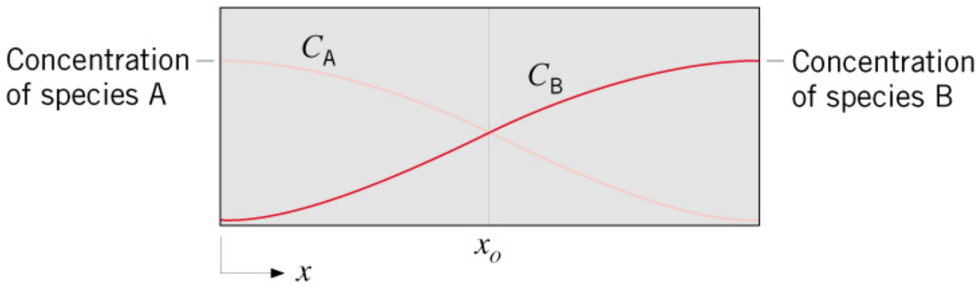
Diffusion is the net transport of substances in a stationary solid or in stagnant fluids or in fluids which are moving only in laminar flow, due to a concentration gradient. It may also be present even in highly developed turbulent flow but near the solid surface .

Advection is the net transport of substances by the moving fluid, and so it cannot happen in solids. It does not include transport of substances by simple diffusion.
Convection is the net transport of substances caused by both advective transport and diffusive transport in fluids.

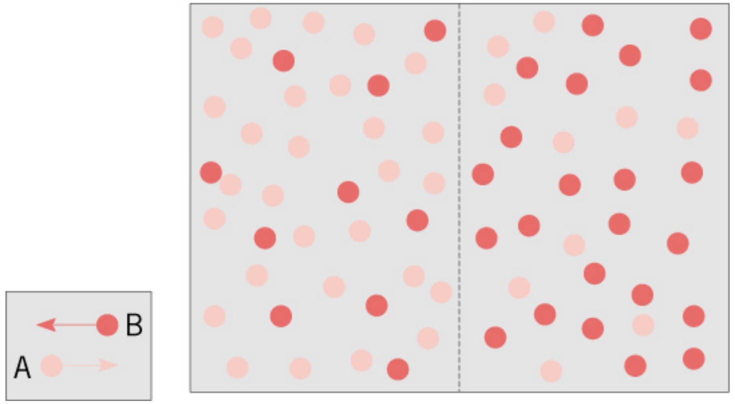
Molecular Diffusion	Convective Mass Transfer
▪ Caused by random <u>microscopic</u> movement of individual molecules in gas/liquid/solid as a result of thermal motion. ▪ Extremely slow. ▪ Occurs in solids and fluids that are stagnant or in laminar flow. ▪ Mass transfer under turbulent-flow but across an interface or near solid surface, the conditions near surface can be assumed laminar. ▪ Mathematically described by Fick's law: $$J^*_{AZ} = -D_{AB}\frac{dc_A}{dz}$$	▪ Caused by random <u>macroscopic</u> fluid bulk motion (dynamic characteristics). ▪ *Orders of magnitude* greater than molecular diffusion. ▪ Involves transport of materials at the interface between moving fluids (liquid-gas) or at interface between a moving fluid and a solid surface (liquid-solid, gas-solid). ▪ Mathematically described in a manner analogous to Newton's law : $$\mathrm{N}_{AZ} = k_C \Delta C_A$$



Consider two species A and B at the same T and p, but initially separated by a partition.



Diffusion in the direction of decreasing concentration dictates net transport of A molecules to the right and B molecules to the left.



In time, uniform concentrations of A and B are approached.

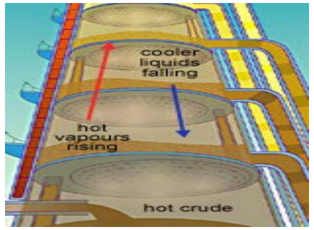
Kinds of Diffusion

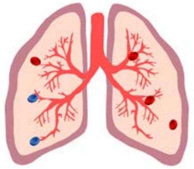
Diffusion Kind	
Ordinary	Due to concentration (Chemical potential) gradient.
Thermal	Due to temperature gradient (CLUSIUS-DICKEL COLUMN).
Pressure	Due to pressure gradient e.g. centrifuges
Forced	Due to unequal external forces acting on the chemical species e.g., ions or charged particles in an electrical field (Nernst-Planck equation).

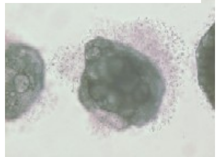
Importance of Mass Transfer: Applications

Mass Transfer

- Industrial
  - Dispersion of flue gases
  - Pollutant sequestration and mitigation
  - Catalysis
  - Distillation / absorption/ extraction / adsorption/ SCF / leaching etc.
  - Air conditioning
- Daily life
  - Inhaling/ exhaling/ oxygen absorption in the lungs
  - Drug release and absorption
  - Sugar dissolution in tea or coffee
  - Moth balls (naphthalene)
  - Sweating







Typically 50 to 90 percent of capital investment in chemical plant is for separations equipment.

Mass and Molar Notation

- Concentration
  - mass concentration ρ_A is the mass of species α per unit volume of solution.
  - Molar concentration $c_A = \rho_A / M_A$ is the number of moles of A per unit volume of solution.
- Fractions
  - mass fraction $\omega_A = \rho_A/\rho$.
  - mole fraction $x_A = c_A/c$.
    - Here $\rho = \Sigma\rho_A$ is the total mass of all species per unit volume of solution, and $c = \Sigma c_A$ is the total number of moles of all species per unit volume of solution.

Table 24.1 Concentrations in a binary mixture of A and B

Molar Liquid Concentrations	Molar Gas Concentrations	Mass Concentrations (Gas or Liquid)
$c = n/V$	$c = n/V = P/RT$	$\rho = m/V$
$c_A = n_A/V$	$c_A = n_A/V = p_A/RT$	$\rho_A = m_A/V$
$c_B = n_B/V$	$c_B = n_B/V = p_B/RT$	$\rho_B = m_B/V$
$x_A = c_A/c$	$y_A = c_A/c = p_A/P$	$w_A = \rho_A/\rho$
$x_B = c_B/c$	$y_B = c_B/c = p_B/P$	$w_B = \rho_B/\rho$
$c = c_A + c_B$	$c = c_A + c_B, P = p_A + p_B$	$\rho = \rho_A + \rho_B$
$1 = x_A + x_B$	$1 = y_A + y_B$	$1 = w_A + w_B$

Example 1

A gas mixture from a hydrocarbon reforming process contains 50% H_2, 40% CO_2, and 10% methane (CH_4) by volume at 400 C (673 K) and 1.5 atm total system pressure. Determine the molar concentration and mass fraction of each species in the mixture, as well as the density of the mixture.

Let $A = H_2$, $B = CO_2$, and $C = CH_4$. Assuming ideal gas behavior, the total molar concentration is

$$c = \frac{P}{RT} = \frac{1.5 \text{ atm}}{(0.08206 \text{ m}^3 \cdot \text{atm/kgmole} \cdot \text{K})(673 \text{ K})} = 2.72 \times 10^{-2} \text{ kgmole/m}^3$$

For an ideal gas, volume percent composition is equivalent to mole percent composition. The molar concentration of species A is

$$c_A = y_A c = (0.50)\left(2.72 \times 10^{-2} \text{ kgmole/m}^3\right) = 1.36 \times 10^{-2} \text{ kgmole/m}^3$$

Similarly, $c_B = 1.10 \times 10^{-2}$ kgmole/m^3, and $c_C = 2.72 \times 10^{-3}$ kgmole/m^3. The mass fraction of each species is determined by the mole fraction and molecular weight of each species:

$$w_A = \frac{y_A M_A}{y_A M_A + y_B M_B + y_C M_C} = \frac{(0.50)(2)}{(0.50)(2) + (0.40)(44) + (0.10)(16)} = 0.0495 \frac{\text{g H}_2}{\text{total g}}$$

Likewise, $w_B = 0.871$, and $w_C = 0.0793$. The mass density of the gas mixture is

$$\begin{aligned} \rho &= \rho_A + \rho_B + \rho_C = c_A M_A + c_B M_B + c_C M_C \\ &= \left(1.36 \times 10^{-2} \frac{\text{kgmole}}{\text{m}^3}\right)\left(\frac{2 \text{ g}}{\text{gmole}}\right) + \left(1.10 \times 10^{-2} \frac{\text{kgmole}}{\text{m}^3}\right)\left(\frac{44 \text{ g}}{\text{gmole}}\right) \\ &\quad + \left(2.72 \times 10^{-3} \frac{\text{kgmole}}{\text{m}^3}\right)\left(\frac{16 \text{ g}}{\text{gmole}}\right) = 0.555 \frac{\text{kg}}{\text{m}^3} \end{aligned}$$

Example 2

A wastewater stream is contaminated with 200 mg/L of dissolved trichloroethylene (TCE) at 20 C, which is below its solubility limit in water. What are the molar concentration (in SI units) and the mole fraction of TCE in the wastewater, assuming a dilute solution? At 20 C, the mass transfer of liquid water is 998.2 kg/m^3 (Appendix I). The molecular weight of the TCE is 131.4 g/gmole, and the molecular weight of water is 18 g/gmole (18 kg/kgmole).

Let species A represent TCE (solute) and species B represent water (solvent). The molar concentration of TCE in the wastewater (c_A) is determined from the mass concentration (ρ_A):

$$c_A = \frac{\rho_A}{M_A} = \frac{200 \text{ mg A/L}}{131.4 \text{ g/gmole}} \frac{1 \text{g}}{1000 \text{ mg}} \frac{1 \text{ kgmole}}{1000 \text{ gmole}} \frac{1000 \text{ L}}{1 \text{ m}^3} = 1.52 \times 10^{-3} \frac{\text{kgmole}}{\text{m}^3}$$

For a dilute solution of TCE (solute A) in water (solvent B), the total molar concentration approximates the molar concentration of the solvent:

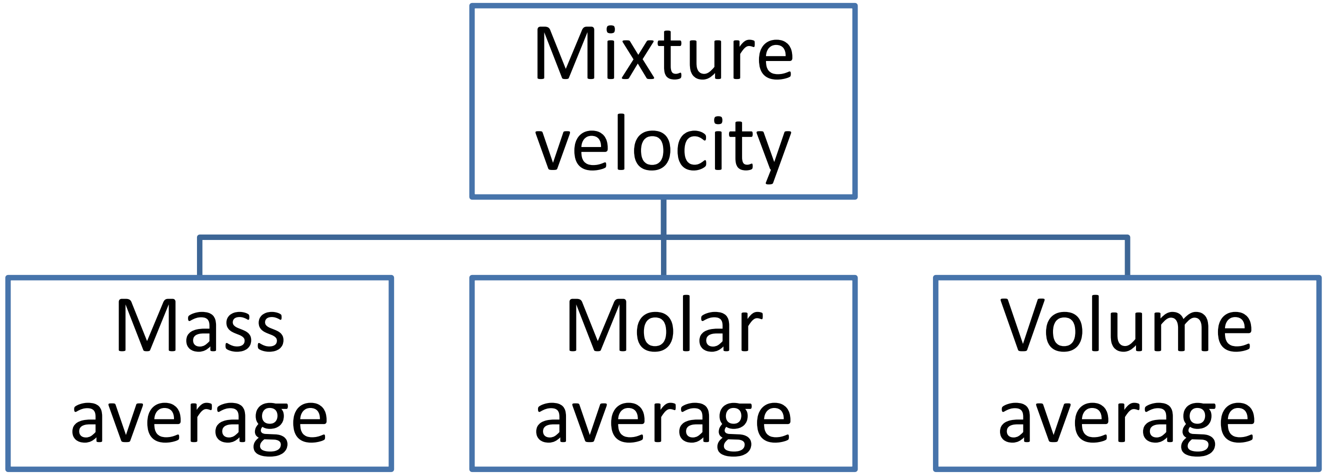
$$c \cong c_B = \frac{\rho_B}{M_B} = \frac{998.3 \text{ kg/m}^3}{18 \text{ kg/kgmole}} = 55.5 \frac{\text{kgmole}}{\text{m}^3}$$

and so the mole fraction (x_A) is

$$x_A = \frac{c_A}{c} = \frac{1.52 \times 10^{-3} \text{ kgmole/m}^3}{55.5 \text{ kgmole/m}^3} = 2.74 \times 10^{-5}$$

Notation for Velocities

- In a diffusing mixture, the various chemical species are moving at different velocities.
  - v_α is the velocity of species α relative to stationary coordinates.
  - Diffusion velocity is the difference between the species velocity and mixture velocity v.



EXAMPLE 2.1 (Estimation of mass average, molar average velocity and volume average velocity): A gas mixture containing 65% NH_3, 8% N_2, 24% H_2 and 3% Ar is flowing through a pipe 25 mm in diameter at a total pressure of 4.0 atm. The velocities of the components are as follows:

NH_3 = 0.03 m/s, N_2 = 0.03 m/s, H_2 = 0.035 m/s and Ar = 0.02 m/s

Calculate the mass average velocity, the molar average velocity and the volume average velocity of the gas mixture.

From Sinha, 2012

Name	i	yi	Mi	vi (m/s)	yivi (m/s)	yiMi	wi	wivi	vi-v	vi-v*	wi(vi-v*)	yi(vi-v)
NH3	1	0.65	17	0.03	0.0195	11.05	0.73814	0.02214	0.00064	-0.0009	-0.00066	0.000417
N2	2	0.08	28	0.03	0.0024	2.24	0.14963	0.00449	0.00064	-0.0009	-0.00013	5.13E-05
H2	3	0.24	2	0.035	0.0084	0.48	0.03206	0.00112	0.00564	0.0041	0.000131	0.001354
Ar	4	0.03	40	0.02	0.0006	1.2	0.08016	0.00160	-0.00936	-0.0109	-0.00087	-0.00028
	S	1	87		0.0309	14.97	1	0.02936	-0.00243	-0.00860	-0.00154	0.00154
					$v^* = \frac{\sum_{\alpha-1}^{N} c_\alpha v_\alpha}{\sum_{\alpha-1}^{N} c_\alpha} = \frac{\sum_{\alpha-1}^{N} c_\alpha v_\alpha}{c} = \sum_{\alpha-1}^{N} x_\alpha v_\alpha$			$v = \frac{\sum_{\alpha-1}^{N} \rho_\alpha v_\alpha}{\sum_{\alpha-1}^{N} \rho_\alpha} = \frac{\sum_{\alpha-1}^{N} \rho_\alpha v_\alpha}{\rho} = \sum_{\alpha-1}^{N} \omega_\alpha v_\alpha$			v-v*	v*-v
											-0.00154	0.00154
					v*			v				

Table 17.7-2 Notation for Velocities in Multicomponent Systems

Basic definitions:		
$\mathbf{v}_\alpha$	velocity of species α with respect to fixed coordinates	(A)
$\mathbf{v} = \sum_{\alpha=1}^{N} \omega_\alpha \mathbf{v}_\alpha$	mass average velocity	(B)
$\mathbf{v}^* = \sum_{\alpha=1}^{N} x_\alpha \mathbf{v}_\alpha$	molar average velocity	(C)
$\mathbf{v}_\alpha - \mathbf{v}$	diffusion velocity of species α with respect to the mass average velocity $\mathbf{v}$	(D)
$\mathbf{v}_\alpha - \mathbf{v}^*$	diffusion velocity of species α with respect to the molar average velocity $\mathbf{v}^*$	(E)
Additional relations:		
$\mathbf{v} - \mathbf{v}^* = \sum_{\alpha=1}^{N} \omega_\alpha(\mathbf{v}_\alpha - \mathbf{v}^*)$ (F)	$\mathbf{v}^* - \mathbf{v} = \sum_{\alpha=1}^{N} x_\alpha(\mathbf{v}_\alpha - \mathbf{v})$	(G)

BSL p. 535

$$v = \frac{\sum_{\alpha=1}^{N} \rho_\alpha v_\alpha}{\sum_{\alpha=1}^{N} \rho_\alpha} = \frac{\sum_{\alpha=1}^{N} \rho_\alpha v_\alpha}{\rho} = \sum_{\alpha=1}^{N} \omega_\alpha v_\alpha$$

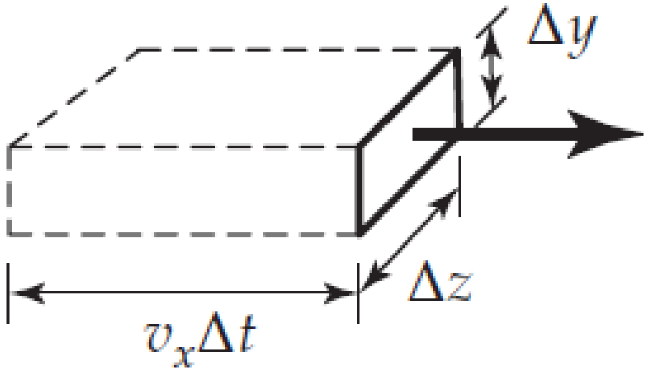
$$v^* = \frac{\sum_{\alpha=1}^{N} c_\alpha v_\alpha}{\sum_{\alpha=1}^{N} c_\alpha} = \frac{\sum_{\alpha=1}^{N} c_\alpha v_\alpha}{c} = \sum_{\alpha=1}^{N} x_\alpha v_\alpha$$

One-Dimensional Convective Fluxes

- Fluxes for a flow in which the fluid is flowing in the x direction only)

- The mass (or molar) flux of a given species is a vector quantity denoting the amount of the particular species, in either mass or molar units, that passes per given increment of time through a unit area normal to the vector.

- The flux may be defined with reference to coordinates that are fixed in space, coordinates that are moving with the mass average velocity, or that are moving with the molar-average velocity.



Flux of mass: $\rho v_x \; [=] \; \frac{M}{L^2 t}$

Flux of momentum: $\rho v_x v_x \; [=] \; \frac{M}{L t^2}$

Flux of kinetic energy: $\frac{1}{2}\rho v_x^2 v_x \; [=] \; \frac{M}{t^3}$

Flux of internal energy: $\rho \hat{U} v_x \; [=] \; \frac{M}{t^3}$

$$\text{Convective Flux} = \left(\text{Quantity/volume}\right)\left(\text{Characteristic Velocity}\right)$$

Molecular (Diffusive) Flux and Fick's First Law of Diffusion

- The molecular flux is defined as

$$\text{Molecular Flux} = \frac{\text{Driving Force}}{\text{Resistance}} = (\text{Diffusivity})(\text{Gradient of quantity/Volume})$$

$$= (\text{Diffusivity})\left(\frac{\text{Quantity/Volume}}{\text{Characteristic length}}\right)$$

$$j_{Ay} = -\rho D_{AB} \frac{d\omega_A}{dy}$$

One-dimensional form of Fick's first law of diffusion.

Valid for any binary solid, liquid, or gas solution, provided that j_{Ay} is defined as the mass flux relative to the mass average velocity of the mixture v_y.

Can be generalized to other dimensions.

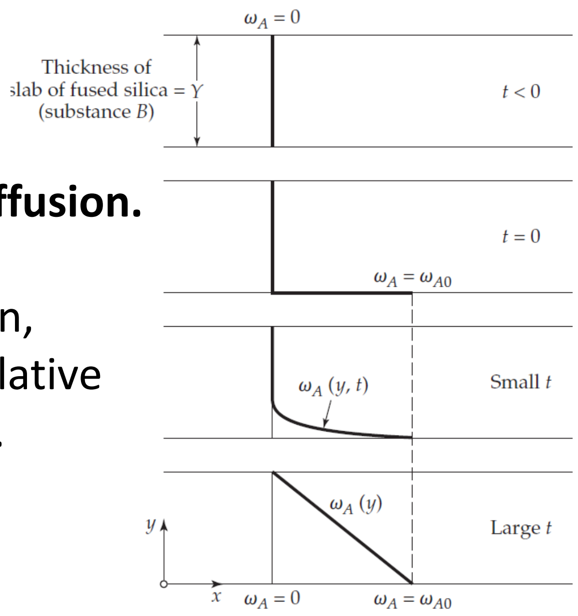


Fig. 17.3-1. Buildup to the steady-state concentration profile for the diffusion of helium (substance A) through fused silica (substance B). The symbol ω_A stands for the mass fraction of helium, and ω_{A0} is the solubility of helium in fused silica, expressed as the mass fraction. See Figs. 1.1-1 and 9.2-1 for analogous momentum and heat-transport situations.

- An empirical relation for molar flux, first postulated by Fick (accordingly often referred to as Fick's first law), can be written as follows for an isothermal, isobaric **binary mixture of *A* and *B*** ***in stagnant media or laminar flow regimes***:

$$J^*_{AZ} = -c_T D_{AB} \frac{dx_A}{dz}$$

J^*_A	is the **molar flux** of component A in the z direction relative to the molar-average velocity in kmol A/s.m^2 (fluxes of molecules)
D_{AB}	is the molecular diffusivity of the molecule A in B in m^2/s
c_T	is the total concentration in kmol (A +B) /m^3.
Z	is the distance of diffusion in m
x_A	is mole fraction of A in the mixture of A and B

Transport Of	Driving Force	Flux Equation	Phenomenological Coefficient	Flux Unit	Common Name
Mass	Concentration gradient	$J_m = -D \cdot \frac{dc}{dx}$	Diffusion coefficient D [m^2/s]	$\left[\frac{kg}{m^2 \cdot s}\right]$	Fick's law of diffusion
Energy/heat	Temperature gradient	$J_h = -k \cdot \frac{dT}{dx}$	Thermal conductivity k [J/(s·K·m)]	$\left[\frac{J}{m^2 \cdot s}\right]$	Fourier's law of heat conduction
Momentum	Velocity gradient	$J_n = -\mu \cdot \frac{dv}{dx}$	Dynamic viscosity μ [Pa·s]	$\left[\frac{kg \cdot (m/s)}{m^2 \cdot s}\right]$	Newton's law of viscosity
Volume	Pressure gradient	$J_v = -L_p \cdot \frac{dP}{dx}$	Permeability coefficient L_p [m^2/(Pa·s)]	$\left[\frac{m^3}{m^2 \cdot s}\right]$	Darcy's law
Electrical	Voltage gradient	$J_e = -\sigma \cdot \frac{dE}{dx}$	Electrical conductance σ [C^2/(s·J·m)]	$\left[\frac{C}{m^2 \cdot s}\right]$	Ohm's law

From Soren Prip Beier, Transport Phenomena, 2013, Bookboon.

Example

A mixture of He and N_2 gas is contained in a pipe at 298 K and 1 atm total pressure which is constant throughout. At one end of the pipe at point 1 the partial pressure p_{A1} of He is 0.6 atm and at the other end 0.2 m p_{A2} = 0.2 atm. Calculate the flux of He at steady state if D_{AB} of the He-N_2 mixture is 0.687 x 10^{-4} m^2/s.

- For steady state the flux J^*_{Az} is constant. Also D_{AB} for gas is constant, then rearranging Eq. (1) and integrating

$$J^*_{Az} \int_{z_1}^{z_2} dz = -D_{AB} \int_{c_{A1}}^{c_{A2}} dc_A$$

$$J^*_{AZ} = \frac{D_{AB}(c_{A1} - c_{A2})}{z_2 - z_1} \qquad (2)$$

Also, from the perfect gas law,

$$p_A V = n_A RT \quad \text{and} \quad c_{A1} = \frac{p_{A1}}{RT} = \frac{n_A}{V}$$

$$J^*_{Az} = \frac{D_{AB}(p_{A1} - p_{A2})}{RT(z_2 - z_1)} \qquad (3)$$

This is the final equation to use, which is in a form easily used for gases. Partial pressures are p_{A1} = 0.6 atm = 0.6 x 1.01325 x 10^5 = 6.04 x 10^4 Pa and p_{A2} = 0.2 atm = 0.2 x 1.01325 x 10^5 = 2.027 x 10^4 Pa. Then, using SI units,

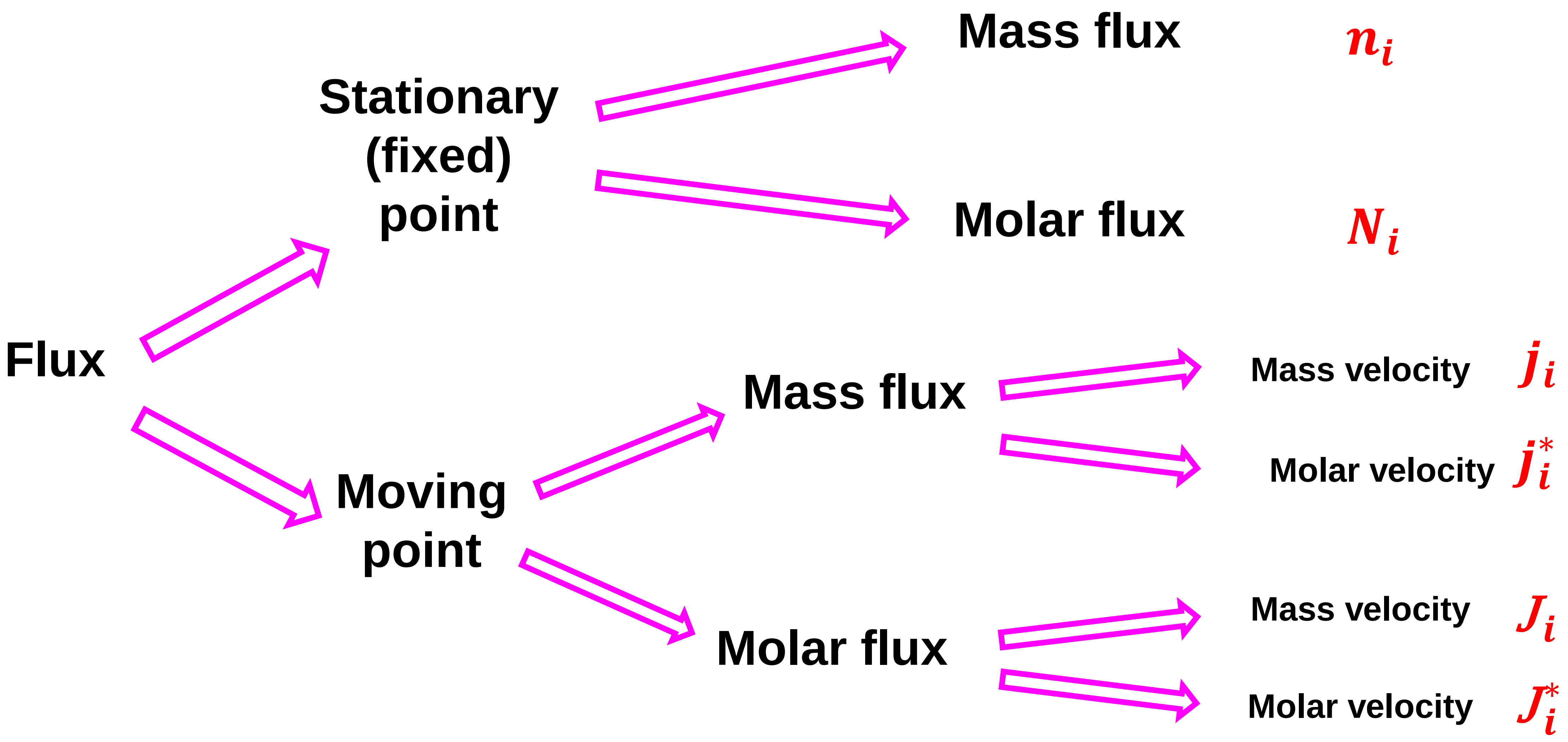
$$J^*_{Az} = \frac{(0.687 \times 10^{-4})(6.08 \times 10^4 - 2.027 \times 10^4)}{8314(298)(0.20 - 0)}$$
$$= 5.63 \times 10^{-6} \text{ kg mol } A/\text{s} \cdot \text{m}^2$$

If pressures in atm are used with SI unit,

$$J^*_{Az} = \frac{(0.687 \times 10^{-4})(0.60 - 0.20)}{(82.06 \times 10^{-3})(298)(0.20 - 0)} = 5.63 \times 10^{-6} \text{ kg mol } A/\text{s} \cdot \text{m}^2$$

Other driving forces (besides concentration differences) for diffusion also occur because of temperature, pressure, electrical potential, and other gradients.

Types of mass transfer fluxes



Diffusivities and Dimensionless Numbers

- Dimensions of L^2/t
  - Momentum diffusivity (kinematic viscosity)

$$\nu = \frac{\mu}{\rho}$$

  - Thermal diffusivity

$$\alpha = \frac{k}{\rho \hat{C}_P}$$

  - Mass diffusivity

$$D_{AB}$$

- Dimensionless
  - Prandtl number

$$\mathrm{Pr} = \frac{\nu}{\alpha} = \frac{\hat{C}_P \mu}{k}$$

  - Schmidt number

$$\mathrm{Sc} = \frac{\nu}{D_{AB}} = \frac{\mu}{\rho D_{AB}}$$

  - Lewis number

$$\mathrm{Le} = \frac{\alpha}{D_{AB}} = \frac{k}{\rho \hat{C}_P D_{AB}}$$

Total Flux and the Peclet Number (Pe)

- The total flux is then the sum of the molecular (diffusive) flux and the convective flux.

$$\text{Total Flux} = \text{Molecular Flux} + \text{Convective Flux}$$

- The ratio of convective to diffusive flux is dimensionless

$$\frac{\text{Convective Flux}}{\text{Molecular Flux}} = \frac{(\text{Characteristic length})(\text{Characteristic velocity})}{\text{Diffusivity}} = \text{Pe}$$

$$\text{Pe}_{\text{MT}} = \frac{L_{ch} v_{ch}}{D_{AB}}, \qquad \text{Pe}_{\text{HT}} = \frac{L_{ch} v_{ch}}{\alpha}, \qquad \text{Pe}_{\text{MomT}} = \frac{L_{ch} v_{ch}}{\nu} = \text{Re}$$

Pe Number as a Classification Tool