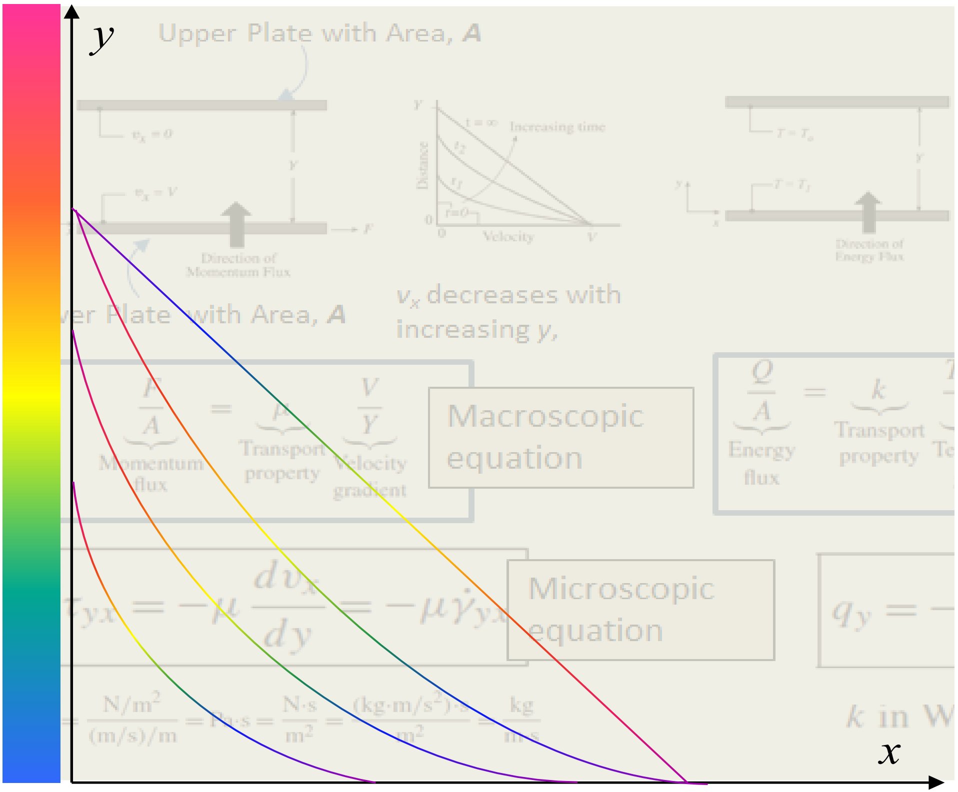


CH403J Modelling & Simulation

Department of Chemical Engineering
SRM Institute of Science and Technology
Kattankulathur

Molecular and Convective Transport

The total flux of any quantity = ***molecular*** + **convective** fluxes

The fluxes arising from *potential gradients* or *driving forces* are called *molecular fluxes*

Molecular fluxes are expressed in the form of *constitutive* (or *phenomenological*) *equations* for **momentum, energy, and mass transport**

Momentum, energy, and mass can also be transported by *bulk fluid motion* or *bulk flow*, and the resulting flux is called *convective flux* **(due to formation of eddies)**

Molecular Transport - *constitutive* (or *phenomenological*) equations

Substances (solid/liquid/or gases) may behave differently when they are subjected to the same gradients.

Constitutive equations identify the *characteristics* of a particular substance.

For instance, if the gradient is ***momentum***, then *viscosity* is defined by the constitutive equation called *Newton's law of viscosity*

If the gradient is ***energy***, then *thermal conductivity* is defined by the constitutive equation called *Fourier's law of heat conduction*

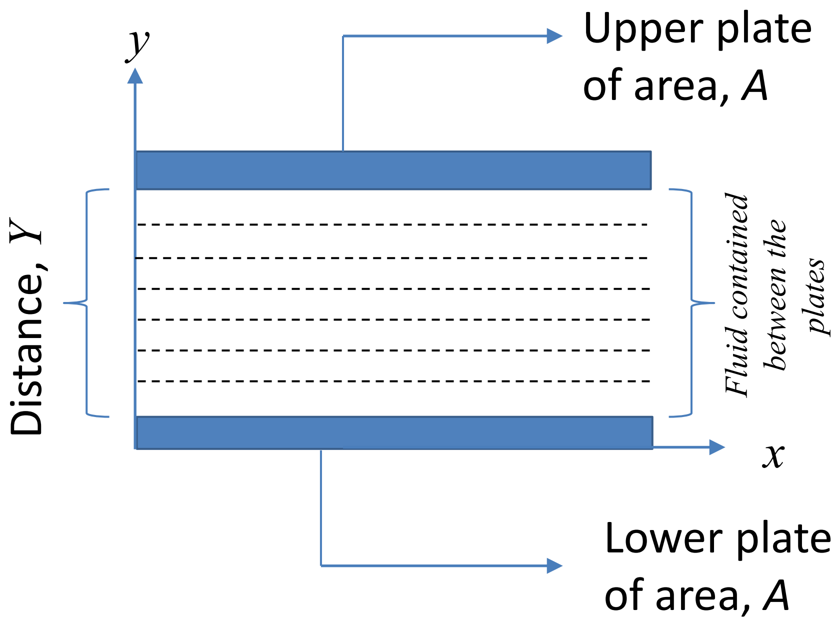
If the gradient is ***concentration***, then *diffusion coefficient* is defined by the constitutive equation called *Fick's first law of diffusion*

Molecular Transport - *constitutive* (or *phenomenological*) equations

Newton's law of viscosity

Consider a fluid contained between two large parallel plates of area *A*, separated by a very small distance *Y* .

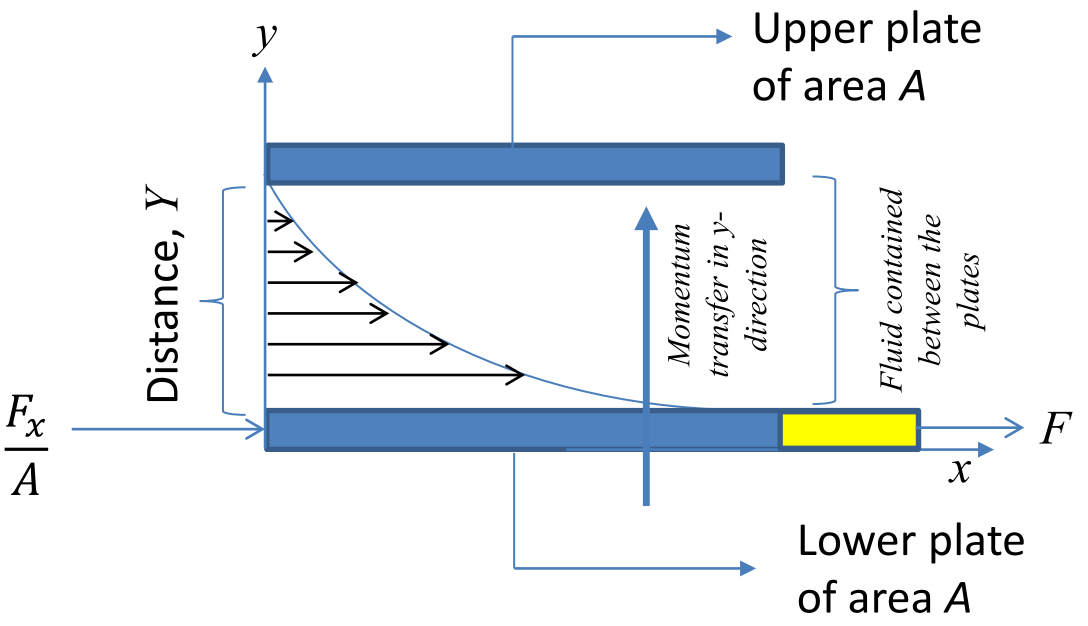
The system is initially at rest



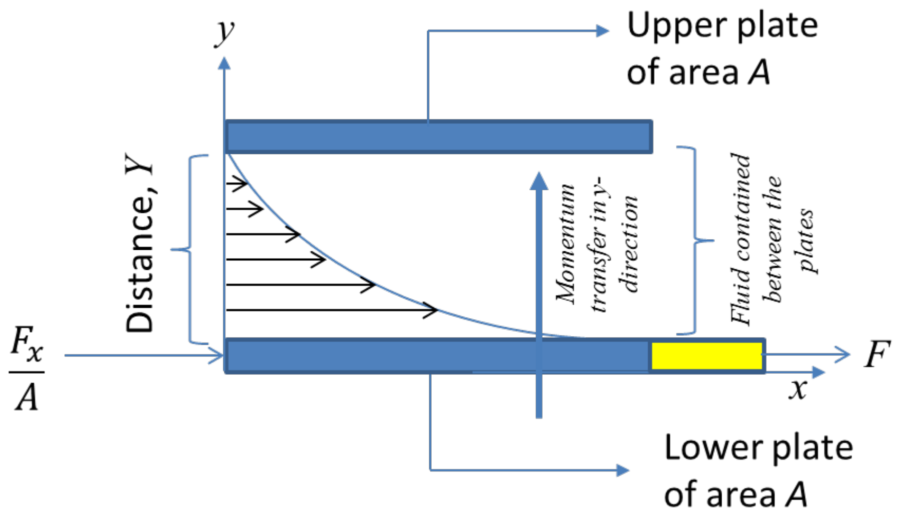
Molecular Transport - *constitutive* (or *phenomenological*) equations

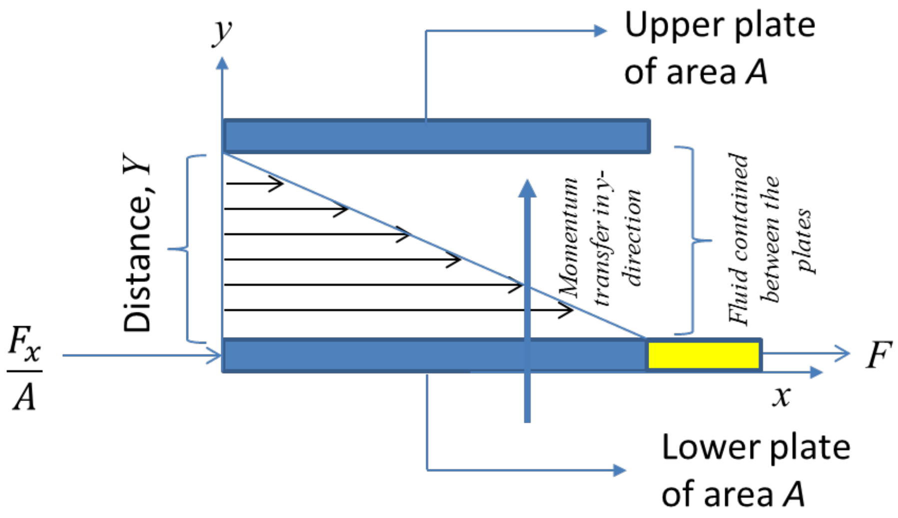
Newton's law of viscosity

The system is initially at rest but at time $t = 0$ the lower plate is set in motion in the x-direction at a constant velocity *V* by applying a force F in the x-direction while the upper plate is kept stationary

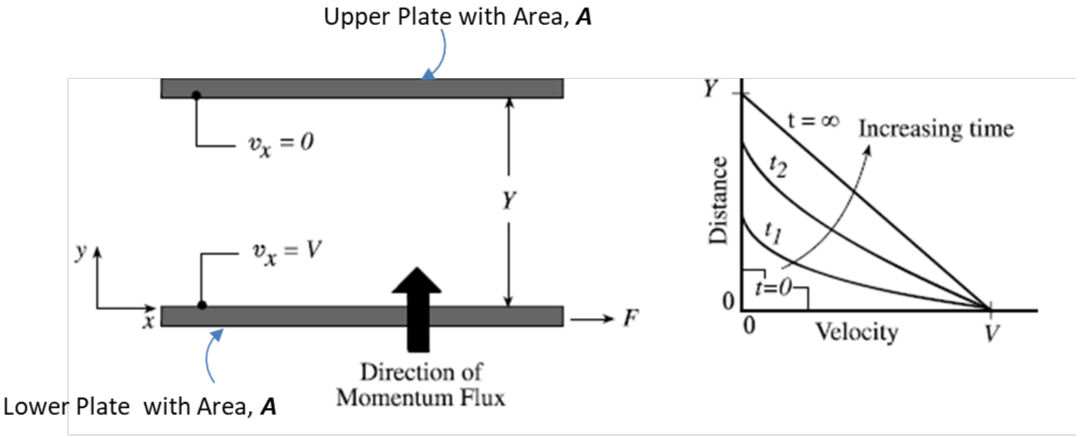


Molecular Transport - *constitutive* (or *phenomenological*) equations





Molecular Transport - *constitutive* (or *phenomenological*) equations



Flow between the parallel plate

Velocity Profile

At time t = 0, the velocity is zero everywhere except at lower plate, which has the velocity *V.* Then the velocity distribution starts as the function of time

Finally at **steady state**, a *linear velocity* distribution is obtained

Molecular Transport - *constitutive* (or *phenomenological*) equations

Experimental results show that the force required to maintain the motion of the lower plate per unit area (or momentum flux) is proportional to the velocity gradient, i.e.,

$$\underbrace{\frac{F}{A}}_{\text{Momentum flux}} = \underbrace{\mu}_{\text{Transport property}} \underbrace{\frac{V}{Y}}_{\text{Velocity gradient}} \qquad (1)$$

and the proportionality constant, μ, is the *viscosity.* Equation (1) is a macroscopic equation. The microscopic form of this equation is given by

$$\boxed{\tau_{yx} = -\mu \frac{dv_x}{dy} = -\mu \dot{\gamma}_{yx}} \qquad (2)$$

which is known as ***Newton's law of viscosity*** and any fluid obeying Eq. (2) is called a ***Newtonian fluid***.

Molecular Transport - *constitutive* (or *phenomenological*) equations

Shear Stress →

$$\tau_{yx} = -\mu \frac{dv_x}{dy} = -\mu \dot{\gamma}_{yx}$$

shear rate

Two subscripts: x represents the direction of force, i.e., F_x , and y represents the direction of the normal to the surface, i.e., A_y, on which the force is acting.

Therefore, τ_{yx} is simply the force per unit area, i.e., F_x/A_y

It is also possible to interpret τ_{yx} as the flux of x-momentum in the y-direction.

Since the velocity gradient is negative, i.e., v_x **decreases with increasing** y

Molecular Transport - *constitutive* (or *phenomenological*) equations

In SI units, shear stress is expressed in N/m^2 (Pa) and velocity gradient in (m/s)/m. Thus, the examination of Eq. (1) indicates that the units of viscosity in SI units are

$$\mu = \frac{N/m^2}{(m/s)/m} = Pa{\cdot}s = \frac{N{\cdot}s}{m^2} = \frac{(kg{\cdot}m/s^2){\cdot}s}{m^2} = \frac{kg}{m{\cdot}s}$$

$1\ Pa{\cdot}s = 10\ P = 10^3\ cP$

Viscosity varies with temperature

For **liquid** *viscosity decreases* with *increasing temperature*
For **gas** *viscosity increases* with *increasing temperature*

Molecular Transport - *constitutive* (or *phenomenological*) equations

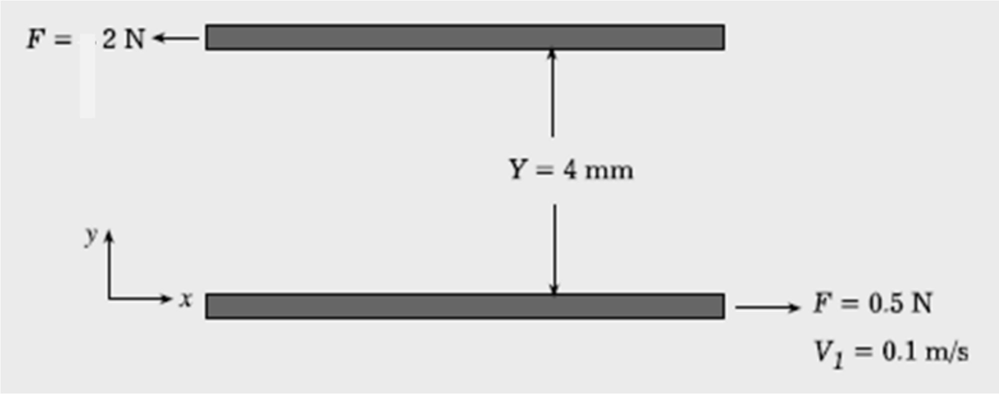
Example 1 (Newton's Law of Viscosity)

A Newtonian fluid with a viscosity of 10 cP is placed between two large parallel plates. The distance between the plates is 4 mm. The lower plate is pulled in the positive x-direction with a force of 0.5 N, while the upper plate is pulled in the negative x-direction with a force of 2 N. Each plate has an area of 2.5 m^2. If the velocity of the lower plate is 0.1 m/s, calculate:

(a) The steady-state momentum flux

(b) The velocity of the upper plate

Molecular Transport - *constitutive* (or *phenomenological*) equations



Given

A = 2.5 m^2

F_1 = 0.5 N

F_2 = 2 N

Y = 4 mm = 4 x 10^{-3} m

Solution

(a) steady state momentum flux

$$\underbrace{\frac{F}{A}}_{\text{Momentum flux}} = \underbrace{\mu}_{\text{Transport property}} \underbrace{\frac{V}{Y}}_{\text{Velocity gradient}}$$

$F/A = (F_1 + F_2)/(A)$ = (0.5 + 2) /(2.5) = **1 N/m^2**

Molecular Transport - *constitutive* (or *phenomenological*) equations

b) Let V_2 be the velocity of the upper plate. From Eq. (2. $\tau_{yx} = -\mu \dfrac{dv_x}{dy}$

$$\tau_{yx} \int_0^Y dy = -\mu \int_{V_1}^{V_2} dv_x \quad \Rightarrow \quad V_2 = V_1 - \frac{\tau_{yx} Y}{\mu} \tag{1}$$

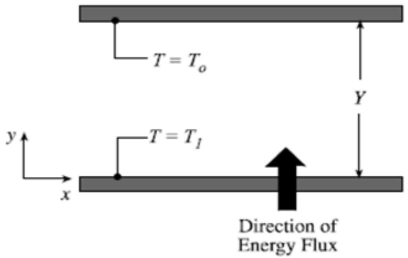
Substitution of the values into Eq. (1) gives

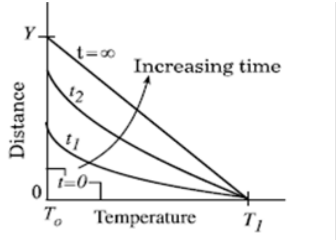
$$V_2 = 0.1 - \frac{(1)(4 \times 10^{-3})}{10 \times 10^{-3}} = -0.3 \text{ m/s} \tag{2}$$

The minus sign indicates that the upper plate moves in the negative x-direction.

Molecular Transport - *constitutive* (or *phenomenological*) equations

Fourier's Law of Heat Conduction





T decreases with increasing *y*,

$$\underbrace{\frac{\dot{Q}}{A}}_{\text{Energy flux}} = \underbrace{k}_{\text{Transport property}} \underbrace{\frac{T_1 - T_o}{Y}}_{\text{Temperature gradient}}$$

$$\boxed{q_y = -k\frac{dT}{dy}}$$

k in W/m·K.

Molecular Transport - *constitutive* (or *phenomenological*) equations

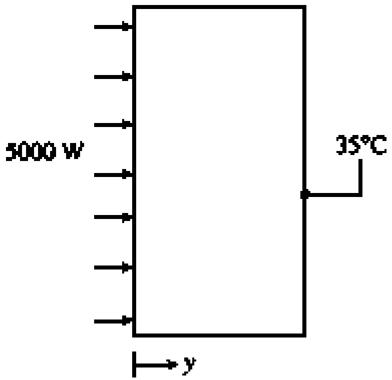
Example 2 (Fourier's Law of Heat Conduction)

One side of a copper slab receives a net heat input at a rate of 5000 W due to radiation. The other face is held at a temperature of 35°C. If steady-state conditions prevail, calculate the surface temperature of the side receiving radiant energy. The surface area of each face is 0.05 m^2, and the slab thickness is 4 cm.

Molecular Transport - *constitutive* (or *phenomenological*) equations

Example 2 (Fourier's Law of Heat Conduction)

Solution



Physical Properties

For copper: $k = 398$ W/m·K

Molecular Transport - *constitutive* (or *phenomenological*) equations

Example 2 (Fourier's Law of Heat Conduction)

System: Copper slab

Under steady conditions with no internal generation, the conservation statement for energy reduces to

$$\text{Rate of energy in} = \text{Rate of energy out} = 5000 \text{ W}$$

Since the slab area across which heat transfer takes place is constant, the heat flux through the slab is also constant, and is given by

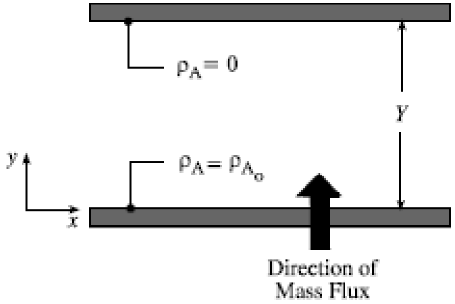
$$q_y = \frac{5000}{0.05} = 100{,}000 \text{ W/m}^2$$

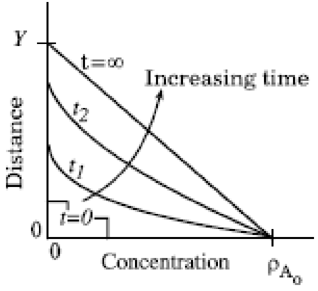
Therefore, the use of Fourier's law of heat conduction, Eq. $\boxed{q_y = -k\,\frac{dT}{dy}}$ gives

$$100{,}000 \int_0^{0.04} dy = -398 \int_{T_o}^{35} dT \quad \Rightarrow \quad T_o = 45.1\,^\circ\text{C}$$

Molecular Transport - *constitutive* (or *phenomenological*) equations

Fick's Law of Diffusion





$$\underbrace{\frac{\dot{m}_A}{A}}_{\substack{\text{Mass}\\ \text{flux of } \mathcal{A}}} = \underbrace{\mathcal{D}_{AB}}_{\substack{\text{Transport}\\ \text{property}}} \underbrace{\frac{\rho_{A_o}}{Y}}_{\substack{\text{Concentration}\\ \text{gradient}}}$$

$$\boxed{J^*_{A_y} = -\mathcal{D}_{AB}\frac{dc_A}{dy}}$$

D_{AB} is in m^2/s

Molecular Transport - *constitutive* (or *phenomenological*) equations

Fick's Law of Diffusion

The diffusion coefficient of gases has an order of magnitude of 10^{-5} m^2/s under atmospheric conditions

Diffusion coefficients for liquids are usually in the order of 10^{-9} m2/s

Diffusion coefficients for solids vary from 10^{-10} to 10^{-14} m^2/s.

Assuming ideal gas behaviour, the pressure and temperature dependence of the diffusion coefficient of gases may be estimated from the relation

$$\mathcal{D}_{AB} \propto \frac{T^{3/2}}{P}$$

Molecular Transport - *constitutive* (or *phenomenological*) equations

Example 3 Fick's Law of Diffusion

Air at atmospheric pressure and 95 °C flows at 20 m/s over a flat plate of naphthalene 80 cm long in the direction of flow and 60 cm wide. Experimental measurements report the molar concentration of naphthalene in the air, c_A, as a function of distance
x from the plate as follows:

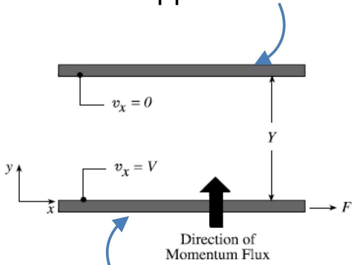
x (cm)	c_A (mol/m^3)
0	0.117
10	0.093
20	0.076
30	0.063
40	0.051
50	0.043

Home Work

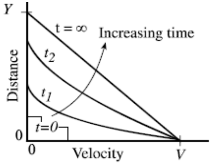
Determine the molar flux of naphthalene from the plate surface under steady conditions.

Molecular Transport - *constitutive* (or *phenomenological*) equations

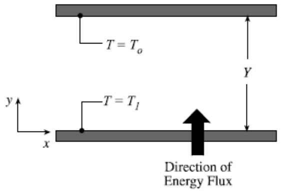
Upper Plate with Area, ***A***

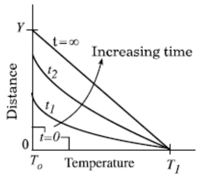


Lower Plate with Area, ***A***

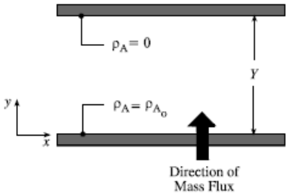


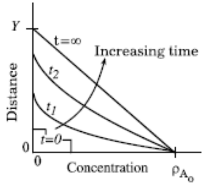
v_x decreases with increasing *y*,





T decreases with increasing *y*,





C decreases with increasing *y*,

$$\underbrace{\frac{F}{A}}_{\text{Momentum flux}} = \underbrace{\mu}_{\text{Transport property}} \underbrace{\frac{V}{Y}}_{\text{Velocity gradient}}$$

Macroscopic equation

$$\underbrace{\frac{\dot{Q}}{A}}_{\text{Energy flux}} = \underbrace{k}_{\text{Transport property}} \underbrace{\frac{T_1 - T_o}{Y}}_{\text{Temperature gradient}}$$

Macroscopic equation

$$\underbrace{\frac{\dot{m}_A}{A}}_{\text{Mass flux of } \mathcal{A}} = \underbrace{\mathcal{D}_{AB}}_{\text{Transport property}} \underbrace{\frac{\rho_{A_o}}{Y}}_{\text{Concentration gradient}}$$

Macroscopic equation

$$\tau_{yx} = -\mu \frac{dv_x}{dy} = -\mu \dot{\gamma}_{yx}$$

Microscopic equation

$$q_y = -k \frac{dT}{dy}$$

Microscopic equation

$$J^*_{A_y} = -\mathcal{D}_{AB} \frac{dc_A}{dy}$$

Microscopic equation

$$\mu = \frac{\mathrm{N/m^2}}{\mathrm{(m/s)/m}} = \mathrm{Pa{\cdot}s} = \frac{\mathrm{N{\cdot}s}}{\mathrm{m^2}} = \frac{\mathrm{(kg{\cdot}m/s^2){\cdot}s}}{\mathrm{m^2}} = \frac{\mathrm{kg}}{\mathrm{m{\cdot}s}}$$

k in W/m·K

D_{AB} is in m^2/s

Molecular Transport - *constitutive* (or *phenomenological*) equations

DIMENSIONLESS NUMBERS

$$\underbrace{\frac{F}{A}}_{\text{Momentum flux}} = \underbrace{\mu}_{\text{Transport property}} \underbrace{\frac{V}{Y}}_{\text{Velocity gradient}}$$

$$\underbrace{\frac{\dot{Q}}{A}}_{\text{Energy flux}} = \underbrace{k}_{\text{Transport property}} \underbrace{\frac{T_1 - T_o}{Y}}_{\text{Temperature gradient}}$$

$$\underbrace{\frac{\dot{m}_A}{A}}_{\text{Mass flux of } \mathcal{A}} = \underbrace{\mathcal{D}_{AB}}_{\text{Transport property}} \underbrace{\frac{\rho_{A_o}}{Y}}_{\text{Concentration gradient}}$$

$$\boxed{\begin{pmatrix}\text{Molecular}\\ \text{flux}\end{pmatrix} = \begin{pmatrix}\text{Transport}\\ \text{property}\end{pmatrix} \begin{pmatrix}\text{Gradient of}\\ \text{driving force}\end{pmatrix}}$$

Molecular Transport - *constitutive* (or *phenomenological*) equations

DIMENSIONLESS NUMBERS

Although the constitutive equations are similar, they are not completely analogous because the transport properties (μ, k, D_{AB}) have different units. These equations can also be expressed in the following forms:

$$\tau_{yx} = -\frac{\mu}{\rho}\frac{d}{dy}(\rho v_x) \qquad \rho = \text{constant} \qquad \rho v_x = \text{momentum/volume}$$

$$q_y = -\frac{k}{\rho \hat{C}_P}\frac{d}{dy}(\rho \hat{C}_P T) \qquad \rho \hat{C}_P = \text{constant} \qquad \rho \hat{C}_P T = \text{energy/volume}$$

$$j_{A_y} = -\mathcal{D}_{AB}\frac{d\rho_A}{dy} \qquad \rho = \text{constant} \qquad \rho_A = \text{mass of } \mathcal{A}\text{/volume}$$

Molecular Transport - *constitutive* (or *phenomenological*) equations

DIMENSIONLESS NUMBERS

Although the constitutive equations are similar, they are not completely analogous because the transport properties (μ, k, D_{AB}) have different units. These equations can also be expressed in the following forms:

Momentum diffusivity or Kinematic viscosity (ν)

$$\tau_{yx} = -\frac{\mu}{\rho}\frac{d}{dy}(\rho v_x) \qquad \rho = \text{constant} \qquad \rho v_x = \text{momentum/volume}$$

$$q_y = -\frac{k}{\rho \hat{C}_p}\frac{d}{dy}(\rho \hat{C}_p T) \qquad \rho \hat{C}_p = \text{constant} \qquad \rho \hat{C}_p T = \text{energy/volume}$$

$$j_{A_y} = -\mathcal{D}_{AB}\frac{d\rho_A}{dy} \qquad \rho = \text{constant} \qquad \rho_A = \text{mass of } \mathcal{A}/\text{volume}$$

Molecular Transport - *constitutive* (or *phenomenological*) equations

DIMENSIONLESS NUMBERS

Although the constitutive equations are similar, they are not completely analogous because the transport properties (μ, k, D_{AB}) have different units. These equations can also be expressed in the following forms:

Thermal diffusivity (α)

$$\tau_{yx} = -\frac{\mu}{\rho}\frac{d}{dy}(\rho v_x) \qquad \rho = \text{constant} \qquad \rho v_x = \text{momentum/volume}$$

$$q_y = -\frac{k}{\rho \hat{C}_p}\frac{d}{dy}(\rho \hat{C}_p T) \qquad \rho \hat{C}_p = \text{constant} \qquad \rho \hat{C}_p T = \text{energy/volume}$$

$$j_{A_y} = -\mathcal{D}_{AB}\frac{d\rho_A}{dy} \qquad \rho = \text{constant} \qquad \rho_A = \text{mass of } \mathcal{A}\text{/volume}$$

Molecular Transport - *constitutive* (or *phenomenological*) equations

DIMENSIONLESS NUMBERS

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$$\tau_{yx} = -\frac{\mu}{\rho}\frac{d}{dy}(\rho v_x) \qquad \rho = \text{constant} \qquad \rho v_x = \text{momentum/volume}$$

$$q_y = -\frac{k}{\rho \hat{C}_P}\frac{d}{dy}(\rho \hat{C}_P T) \qquad \rho \hat{C}_P = \text{constant} \qquad \rho \hat{C}_P T = \text{energy/volume}$$

$$j_{A_y} = \boxed{-\mathcal{D}_{AB}}\frac{d\rho_A}{dy} \qquad \rho = \text{constant} \qquad \rho_A = \text{mass of } \mathcal{A}/\text{volume}$$

Mass diffusivity

Molecular Transport - *constitutive* (or *phenomenological*) equations

DIMENSIONLESS NUMBERS

Although the constitutive equations are similar, they are not completely analogous because the transport properties (μ, k, D_{AB}) have different units. These equations can also be expressed in the following forms:

$$\tau_{yx} = -\frac{\mu}{\rho}\frac{d}{dy}(\rho v_x) \qquad \rho = \text{constant} \qquad \rho v_x = \text{momentum/volume}$$

$$q_y = -\frac{k}{\rho \hat{C}_P}\frac{d}{dy}(\rho \hat{C}_P T) \qquad \rho \hat{C}_P = \text{constant} \qquad \rho \hat{C}_P T = \text{energy/volume}$$

$$j_{A_y} = -\mathcal{D}_{AB}\frac{d\rho_A}{dy} \qquad \rho = \text{constant} \qquad \rho_A = \text{mass of } \mathcal{A}/\text{volume}$$

Molecular Transport - *constitutive* (or *phenomenological*) equations

DIMENSIONLESS NUMBERS

Analogous terms in constitutive equations for momentum, energy, and mass (or mole) transfer in one-dimension

	Momentum	Energy	Mass	Mole
Molecular flux	τ_{yx}	q_y	j_{A_y}	$J^*_{A_y}$
Transport property	μ	k	$\mathcal{D}_{AB}$	$\mathcal{D}_{AB}$
Gradient of driving force	$\frac{dv_x}{dy}$	$\frac{dT}{dy}$	$\frac{d\rho_A}{dy}$	$\frac{dc_A}{dy}$
Diffusivity	ν	α	$\mathcal{D}_{AB}$	$\mathcal{D}_{AB}$
Quantity/Volume	ρv_x	$\rho \hat{C}_p T$	ρ_A	c_A
Gradient of Quantity/Volume	$\frac{d(\rho v_x)}{dy}$	$\frac{d(\rho \hat{C}_p T)}{dy}$	$\frac{d\rho_A}{dy}$	$\frac{dc_A}{dy}$

Note that the terms v, α, and D_{AB} all have the same units, m^2/s

Molecular Transport - *constitutive* (or *phenomenological*) equations

$$\boxed{\tau_{yx} = -\mu \frac{dv_x}{dy} = -\mu \dot{\gamma}_{yx}}$$

$$\tau_{yx} = -\frac{\mu}{\rho} \frac{d}{dy}(\rho v_x) \qquad \rho = \text{constant} \qquad \rho v_x = \text{momentum/volume}$$

$$\boxed{q_y = -k \frac{dT}{dy}}$$

$$q_y = -\frac{k}{\rho \hat{C}_p} \frac{d}{dy}(\rho \hat{C}_p T) \qquad \rho \hat{C}_p = \text{constant} \qquad \rho \hat{C}_p T = \text{energy/volume}$$

$$\boxed{J^*_{A_y} = -\mathcal{D}_{AB} \frac{dc_A}{dy}}$$

$$j_{A_y} = -\mathcal{D}_{AB} \frac{d\rho_A}{dy} \qquad \rho = \text{constant} \qquad \rho_A = \text{mass of } \mathcal{A}\text{/volume}$$

$$\boxed{\begin{pmatrix}\text{Molecular}\\ \text{flux}\end{pmatrix} = \begin{pmatrix}\text{Transport}\\ \text{property}\end{pmatrix}\begin{pmatrix}\text{Gradient of}\\ \text{driving force}\end{pmatrix}}$$

$$\boxed{\begin{pmatrix}\text{Molecular}\\ \text{flux}\end{pmatrix} = (\text{Diffusivity})\begin{pmatrix}\text{Gradient of}\\ \text{Quantity/Volume}\end{pmatrix}}$$

Molecular Transport - *constitutive* (or *phenomenological*) equations

The ratio of momentum diffusivity to thermal diffusivity gives the *Prandtl number*, Pr:

$$\text{Prandtl number} = \text{Pr} = \frac{\nu}{\alpha} = \frac{\widehat{C}_P \mu}{k}$$

The Prandtl number is a function of temperature and pressure. However, its dependence on temperature, at least for liquids, is much stronger. The order of magnitude of the Prandtl number for gases and liquids can be estimated as

$$\text{Pr} = \frac{(10^3)(10^{-5})}{10^{-2}} = 1 \qquad \text{for gases}$$

$$\text{Pr} = \frac{(10^3)(10^{-3})}{10^{-1}} = 10 \qquad \text{for liquids}$$

Molecular Transport - *constitutive* (or *phenomenological*) equations

The ratio of momentum to mass diffusivities gives the *Schmidt number*, Sc:

$$\text{Schmidt number} = \text{Sc} = \frac{\nu}{\mathcal{D}_{AB}} = \frac{\mu}{\rho \mathcal{D}_{AB}}$$

The order of magnitude of the Schmidt number for gases and liquids can be estimated as

$$\text{Sc} = \frac{10^{-5}}{(1)(10^{-5})} = 1 \qquad \text{for gases}$$

$$\text{Sc} = \frac{10^{-3}}{(10^{3})(10^{-9})} = 10^{3} \qquad \text{for liquids}$$

Molecular Transport - *constitutive* (or *phenomenological*) equations

Finally, the ratio of α to $\mathcal{D}_{AB}$ gives the *Lewis number*, Le:

$$\text{Lewis number} = \text{Le} = \frac{\alpha}{\mathcal{D}_{AB}} = \frac{k}{\rho \hat{C}_P \mathcal{D}_{AB}} = \frac{\text{Sc}}{\text{Pr}}$$

Convective Transport

$$\boxed{\begin{pmatrix}\text{Convective}\\ \text{flux}\end{pmatrix} = (\text{Quantity/Volume})\begin{pmatrix}\text{Characteristic}\\ \text{velocity}\end{pmatrix}}$$

For a single phase system composed of *n* components, the general definition of a characteristic velocity is given by

$$v_{ch} = \sum_{i}^{n} \beta_i \, v_i$$

where β_i is the weighting factor and v_i is the velocity of a constituent.

Convective Transport

Common characteristic velocities

Characteristic Velocity	Weighting Factor	Formulation
Mass average	Mass fraction (ω_i)	$v = \sum_i \omega_i v_i$
Molar average	Mole fraction (x_i)	$v^* = \sum_i x_i v_i$
Volume average	Volume fraction ($c_i \overline{V}_i$)	$v^{\blacksquare} = \sum_i c_i \overline{V}_i v_i$

Convective Transport

Since the total flux of any quantity is the sum of its molecular and convective fluxes,

$$\begin{pmatrix}\text{Total}\\ \text{flux}\end{pmatrix} = \underbrace{\begin{pmatrix}\text{Transport}\\ \text{property}\end{pmatrix}\begin{pmatrix}\text{Gradient of}\\ \text{driving force}\end{pmatrix}}_{\text{Molecular flux}} + \underbrace{\left(\frac{\text{Quantity}}{\text{Volume}}\right)\begin{pmatrix}\text{Characteristic}\\ \text{velocity}\end{pmatrix}}_{\text{Convective flux}}$$

or,

$$\begin{pmatrix}\text{Total}\\ \text{flux}\end{pmatrix} = \underbrace{(\text{Diffusivity})\begin{pmatrix}\text{Gradient of}\\ \text{Quantity/Volume}\end{pmatrix}}_{\text{Molecular flux}} + \underbrace{\left(\frac{\text{Quantity}}{\text{Volume}}\right)\begin{pmatrix}\text{Characteristic}\\ \text{velocity}\end{pmatrix}}_{\text{Convective flux}}$$

the ratio of the convective flux to the molecular flux is given by

$$\frac{\text{Convective flux}}{\text{Molecular flux}} = \frac{(\text{Quantity/Volume})(\text{Characteristic velocity})}{(\text{Diffusivity})(\text{Gradient of Quantity/Volume})} \qquad (1)$$

Convective Transport

$$\frac{\text{Convective flux}}{\text{Molecular flux}} = \frac{(\text{Quantity/Volume})(\text{Characteristic velocity})}{(\text{Diffusivity})(\text{Gradient of Quantity/Volume})}$$

"**Gradient of Quantity/Volume**" can be expressed as

$$\text{Gradient of Quantity/Volume} = \frac{\text{Difference in Quantity/Volume}}{\text{Characteristic length}} \qquad (2)$$

The use of Eq. (2) and (1)

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

The ratio of the convective flux to the molecular flux is known as the *Peclet number*, Pe

Convective Transport

The ratio of the convective flux to the molecular flux is known as the *Peclet number*, Pe. Therefore, Peclet numbers for heat and mass transfers are

$$\mathrm{Pe_H} = \frac{v_{ch} L_{ch}}{\alpha}$$

$$\mathrm{Pe_M} = \frac{v_{ch} L_{ch}}{\mathcal{D}_{AB}}$$

Hence, the total flux of any quantity is given by

$$\text{Total flux} = \begin{cases} \text{Molecular flux} & \mathrm{Pe} \ll 1 \\ \text{Molecular flux} + \text{Convective flux} & \mathrm{Pe} \simeq 1 \\ \text{Convective flux} & \mathrm{Pe} \gg 1 \end{cases}$$

Rate of mass entering or leaving the system

The mass flow rate of species i entering and/or leaving the system, $\dot{m}_i$, is expressed as

$$\dot{m}_i = \Bigg[\underbrace{\begin{pmatrix} \text{Mass} \\ \text{Diffusivity} \end{pmatrix} \begin{pmatrix} \text{Gradient of} \\ \text{Mass of } i/\text{Volume} \end{pmatrix}}_{\text{Molecular mass flux of species } i} + \underbrace{\left(\frac{\text{Mass of } i}{\text{Volume}} \right) \begin{pmatrix} \text{Characteristic} \\ \text{velocity} \end{pmatrix}}_{\text{Convective mass flux of species } i} \Bigg] \begin{pmatrix} \text{Flow} \\ \text{area} \end{pmatrix}$$

$\mathrm{Pe_M} \gg 1$ The above equation simplifies into

$$\dot{m}_i = \left(\frac{\text{Mass of } i}{\text{Volume}} \right) \begin{pmatrix} \text{Average} \\ \text{velocity} \end{pmatrix} \begin{pmatrix} \text{Flow} \\ \text{area} \end{pmatrix}$$

or,

$$\boxed{\dot{m}_i = \rho_i \langle v \rangle A = \rho_i Q}$$

Rate of mass entering or leaving the system

The total mass flow rate, $\dot{m}$, entering and/or leaving the system by a conduit in the form

$$\boxed{\dot{m} = \rho\langle v\rangle A = \rho Q}$$

On a molar basis,

$$\boxed{\dot{n}_i = c_i\langle v\rangle A = c_i Q}$$

$$\boxed{\dot{n} = c\langle v\rangle A = cQ}$$

Rate of Energy Entering and/or Leaving the System

The rate of energy entering and/or leaving the system, $\dot{E}$, is expressed as

$$\dot{E} = \left[\underbrace{\begin{pmatrix} \text{Thermal} \\ \text{diffusivity} \end{pmatrix} \begin{pmatrix} \text{Gradient of} \\ \text{Energy/Volume} \end{pmatrix}}_{\text{Molecular energy flux}} + \underbrace{\left(\frac{\text{Energy}}{\text{Volume}} \right) \begin{pmatrix} \text{Characteristic} \\ \text{velocity} \end{pmatrix}}_{\text{Convective energy flux}} \right] \begin{pmatrix} \text{Flow} \\ \text{area} \end{pmatrix}$$

As in the case of mass, energy may enter or leave the system by two means:

- By inlet and/or outlet streams,
- By exchange of energy between the system and its surroundings through the boundaries of the system in the form of heat and work.

Rate of Energy Entering and/or Leaving the System

$\mathrm{Pe_M} \gg 1$

$$\dot{E} = \Bigg[\underbrace{\begin{pmatrix}\text{Thermal}\\ \text{diffusivity}\end{pmatrix}\begin{pmatrix}\text{Gradient of}\\ \text{Energy/Volume}\end{pmatrix}}_{\text{Molecular energy flux}} + \underbrace{\left(\frac{\text{Energy}}{\text{Volume}}\right)\begin{pmatrix}\text{Characteristic}\\ \text{velocity}\end{pmatrix}}_{\text{Convective energy flux}} \Bigg] \begin{pmatrix}\text{Flow}\\ \text{area}\end{pmatrix}$$

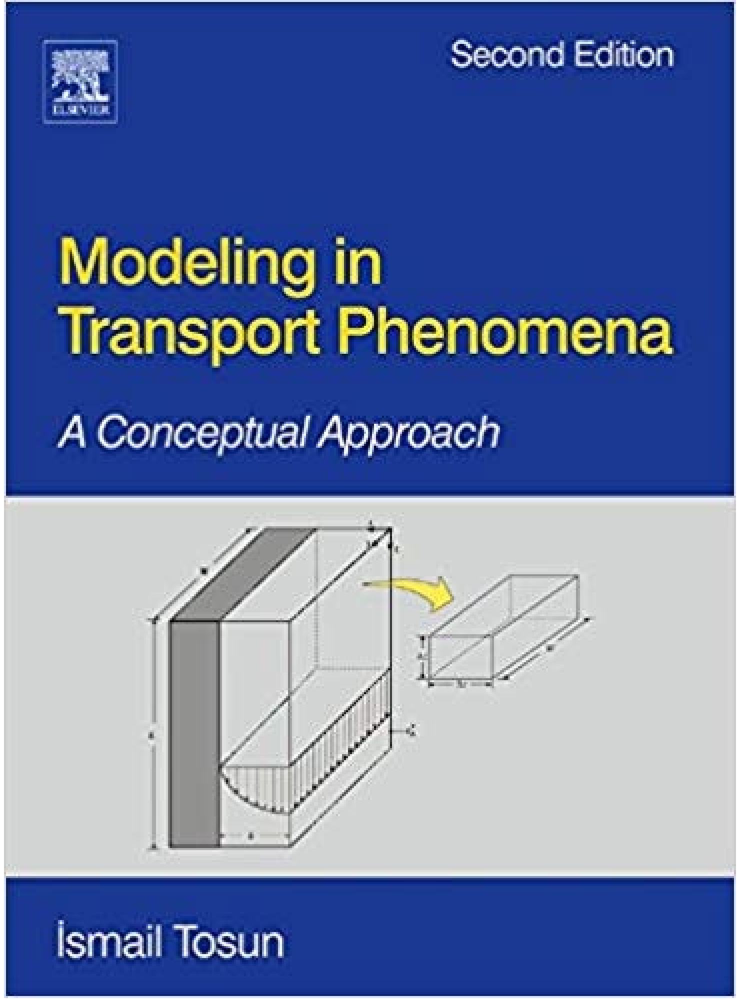
The total flux equation

$$\dot{E} = \left(\frac{\text{Energy}}{\text{Volume}}\right)\begin{pmatrix}\text{Average}\\ \text{velocity}\end{pmatrix}\begin{pmatrix}\text{Flow}\\ \text{area}\end{pmatrix}$$

Energy per unit volume, on the other hand, is expressed as the product of energy per unit mass, $\widehat{E}$, and mass per unit volume, i.e., density, such that Eq. (2.4-16) becomes

$$\dot{E} = \left(\frac{\text{Energy}}{\text{Mass}}\right)\underbrace{\left(\frac{\text{Mass}}{\text{Volume}}\right)\begin{pmatrix}\text{Average}\\ \text{velocity}\end{pmatrix}\begin{pmatrix}\text{Flow}\\ \text{area}\end{pmatrix}}_{\text{Mass flow rate}} = \widehat{E}\,\dot{m}$$

References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