EKC314: TRANSPORT PHENOMENA
Core Course for
B.Eng.(Chemical Engineering)
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1. Introduction and Concepts

2. Momentum Transport
   - Viscosity and mechanism of momentum transport
   - Newtonian and non-newtonian fluids
   - Flux and gradients
   - Velocity distribution in laminar and turbulent flows
   - Boundary layer
   - Velocity distribution with more than one independent variables
3. Equation of changes in Isothermal Systems;
   6 Interphase transport in isothermal system.
   6 Macroscopic balances for isothermal systems.
Introduction and Concepts

What are Transport Phenomena?
1. Fluid dynamics
2. Heat transfer
3. Mass transfer

They should be studied together since:
1. they occur simultaneously
2. basic equations that described the 3 transport phenomena are closely related
3. mathematical tools required are very similar
4. molecular mechanisms underlying various transport phenomena are very closely related
Introduction and Concepts

Macroscopic level
- Write down balance equation; macroscopic balances.
- Equations should describe mass, momentum, energy and angular momentum within the system.
- No need to understand the details of the system.

Microscopic level
- Examination of the fluid mixture in a small region within the equipment.
- Can write down the equation of change that describe mass, momentum, energy and angular momentum change within the small region.
- Aim is to get information about velocity, temperature, pressure and concentration profile within the system.

Molecular level
- To seek a fundamental understanding of the mechanism of mass, momentum, energy and angular momentum in terms of molecular structure and intermolecular forces.
- Involve some theoretical physics and physical chemistry work.
Introduction and Concepts

Mixture of gases

Macroscopic

Heat added to the system

Microscopic

Molecular
Introduction and Concepts

The flow of fluid are studied in 3 different parts which consist of:

1. flow of pure fluids at constant temperature-with emphasis on **viscous** and **convective** momentum transport
2. flow of pure fluids with varying temperature-with emphasis on **conductive**, **convective** and **radiative** energy transport
3. flow of fluid mixtures with varying composition-with emphasis on **diffusive** and **convective** mass transport
Conservation Laws (mass):

- Consider two colliding diatomic molecules (N$_2$ and O$_2$).
- The **conservation of mass** can be written as;

  \[ m_N + m_O = m'_N + m'_O \]

for a system with no chemical reaction;

\[ m_N = m'_N \]

and

\[ m_O = m'_O \]
Introduction and Concepts

Conservation Laws (momentum):

According to the law of conservation of momentum, the sum of the momenta of all atoms before collision must equal that after the collision.

The conservation of momentum can be written as:

\[ m_{N_1} \dot{r}_{N_1} + m_{N_2} \dot{r}_{N_2} + m_{O_1} \dot{r}_{O_1} + m_{O_2} \dot{r}_{O_2} \]

\[ = m'_{N_1} \dot{r}'_{N_1} + m'_{N_2} \dot{r}'_{N_2} + m'_{O_1} \dot{r}'_{O_1} + m'_{O_2} \dot{r}'_{O_2} \]
Conservation Laws (momentum):

- $\mathbf{r}_{N1}$ is the position vector for atom 1 of molecule N and $\dot{\mathbf{r}}_{N1}$ is its velocity.
- It can be written as:

$$\mathbf{r}_{N1} = \mathbf{r}_N + \mathbf{R}_{N1}$$

- $\mathbf{r}_{N1}$ is the sum of the position vector for the centre of mass and the position vector of the atom w.r.t the centre of mass.
Conservation Laws (momentum):

- Also $R_{N_2} = -R_{N_1}$
- Then the conservation equation can be simplified as:

$$m_N \dot{r}_N + m_O \dot{r}_O = m_N \dot{r}'_N + m_O \dot{r}'_O$$
Introduction and Concepts

How to study Transport Phenomena?

1. Read the text with pencil and paper in hand-work through details of the mathematical developments.
2. Refer back to any maths textbook just to brush up on calculus, differential equations, vectors etc.
3. Make a point to give a physical interpretation of key results-get into habit of relating physical ideas to the equations.
4. Ask whether results seem reasonable. If they do not agree with intuition, it is important to find out which is correct.
5. Make a habit to check the dimensions of all results. This is a very good way to locate errors in derivations.
Recap: Vector Calculus

If given a vector of a form:

\[ \mathbf{a} = [a_1, a_2, a_3] = a_1 \mathbf{i} + a_2 \mathbf{j} + a_3 \mathbf{k} \]

consists of the real vector space \( \mathbb{R}^3 \) with vector addition defined as:

\[ [a_1, a_2, a_3] + [b_1, b_2, b_3] = [a_1 + b_1, a_2 + b_2, a_3 + b_3] \]

and scalar multiplication defined by:

\[ c[a_1, a_2, a_3] = [ca_1, ca_2, ca_3] \]
The **dot product** of two vectors is defined by;

\[ \mathbf{a} \cdot \mathbf{b} = |\mathbf{a}| |\mathbf{b}| \cos \gamma = a_1 b_1 + a_2 b_2 + a_3 b_3 \]

where \( \gamma \) is the angle between \( \mathbf{a} \) and \( \mathbf{b} \). This gives the **norm** or **length** \( |\mathbf{a}| \) of \( \mathbf{a} \) with a formula;

\[ |\mathbf{a}| = \sqrt{\mathbf{a} \cdot \mathbf{a}} = \sqrt{a_1^2 + a_2^2 + a_3^2} \]

If \( \mathbf{a} \cdot \mathbf{b} = 0 \) therefore \( \mathbf{a} \) and \( \mathbf{b} \) orthogonal.
Example of a dot product is given by:

\[ W = \mathbf{p} \cdot \mathbf{d} \]

which is work done by a force \( \mathbf{p} \) in a displacement \( \mathbf{d} \).
Introduction and Concepts

The **cross product** \( \mathbf{v} = \mathbf{a} \times \mathbf{b} \) is a vector of length;

\[ |\mathbf{a} \times \mathbf{b}| = |\mathbf{a}||\mathbf{b}| \sin \gamma \]

and perpendicular to both \( \mathbf{a} \) and \( \mathbf{b} \) such that \( \mathbf{a}, \mathbf{b}, \mathbf{v} \) form a right-handed triple.

This can also be written in the form of;

\[ \mathbf{a} \times \mathbf{b} = \begin{pmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{pmatrix} \]

The **cross product** is *anticommutative* \( \mathbf{a} \times \mathbf{b} = -\mathbf{b} \times \mathbf{a} \) and not associative.
For a vector function given by

\[ \mathbf{v}(t) = [v_1(t), v_2(t), v_3(t)] = v_1(t)i + v_2(t)j + v_3(t)k \]

Then the derivative is;

\[ \mathbf{v}' = \frac{d\mathbf{v}}{dt} = \lim_{\Delta t \to 0} \frac{\mathbf{v}(t + \Delta t) - \mathbf{v}(t)}{\Delta t} \]

therefore;

\[ \mathbf{v}' = [v'_1, v'_2, v'_3] = v'_1i + v'_2j + v'_3k \]
Introduction and Concepts

Vector function $\mathbf{r}(t)$ can be used to represent a curve $C$ in space.

Then $\mathbf{r}(t)$ associates with each $t = t_0$ in some interval $a < t < b$ the point of $C$ with position vector $\mathbf{r}(t_0)$.

The derivative $\mathbf{r}'(t)$ is a tangent vector of $C$.

If a vector in a Cartesian coordinate is given by;

$$\mathbf{v}(x, y, z) = [v_1(x, y, z), v_2(x, y, z), v_3(x, y, z)]$$

$$= v_1(x, y, z)\mathbf{i} + v_2(x, y, z)\mathbf{j} + v_3(x, y, z)\mathbf{k}$$
Therefore, the partial derivative of $v$ can be obtained by:

\[
\frac{\partial v}{\partial x} = \left( \frac{\partial v_1}{\partial x}, \frac{\partial v_2}{\partial x}, \frac{\partial v_3}{\partial x} \right)
\]

\[
= \frac{\partial v_1}{\partial x} \mathbf{i} + \frac{\partial v_2}{\partial x} \mathbf{j} + \frac{\partial v_3}{\partial x} \mathbf{k}
\]
Gradient of a function $f$ can be written as;

$$\text{grad } f = \nabla f = \left[ \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right]$$

Therefore, using the operation, the **directional derivative** of $f$ in a direction of a unit vector $b$ can be obtained by;

$$D_b f = \frac{df}{ds} = b \cdot \nabla f$$
**Introduction and Concepts**

- **Divergence** of a vector function \( \mathbf{v} \) can be written as:

\[
\text{div } \mathbf{v} = \nabla \cdot \mathbf{v} = \frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y} + \frac{\partial v_3}{\partial z}
\]

- And the curl of \( \mathbf{v} \) is given as:

\[
\text{curl } \mathbf{v} = \nabla \times \mathbf{v} = \begin{pmatrix}
\mathbf{i} & \mathbf{j} & \mathbf{k} \\
\frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\
v_1 & v_2 & v_3
\end{pmatrix}
\]
Some basic formula for grad, div and curl;

Grad:

\[ \nabla (fg) = f \nabla g + g \nabla f \]
\[ \nabla (f/g) = (1/g^2)(g \nabla f - f \nabla g) \]

Div:

\[ \text{div}(fv) = f \text{div} \quad v + v \cdot \nabla f \]
\[ \text{div}(f \nabla g) = f \nabla^2 g + \nabla f \cdot \nabla g \]
Introduction and Concepts

Div and Grad (Laplacian):

\[ \nabla^2 f = \text{div}(\nabla f) \]

\[ \nabla^2 (fg) = g\nabla^2 f + 2\nabla f \cdot \nabla g + f\nabla^2 g \]

Div and Curl:

\[ \text{curl}(fv) = \nabla f \times v + f\text{curl }v \]

\[ \text{div}(u \times v) = v \cdot \text{curl }u - u \cdot \text{curl }v \]
Introduction and Concepts

Extra:

\[ \text{curl}(\nabla f) = 0 \]
\[ \text{div}(\text{curl } \mathbf{v}) = 0 \]
Example 1:
Let a particle A of mass \( M \) be fixed at point \( P_0 \) and let a particle B of mass \( m \) be free to take up various positions \( \mathcal{P} \) in space. Then A attracts B. According to **Newton’s Law of Gravitation**, the corresponding gravitational force \( \mathbf{p} \) is directed from \( \mathcal{P} \) to \( P_0 \) and its magnitude is proportional to \( \frac{1}{r^2} \), where \( r \) is the distance between \( \mathcal{P} \) and \( P_0 \). This can be written as;

\[
| \mathbf{p} | = \frac{c}{r^2}
\]
Hence \( \mathbf{p} \) defines a vector field in space. Using Cartesian coordinates, such that \( P_0(x_0, y_0, z_0) \) and \( P(x, y, z) \), therefore the distance \( r \) can be determined as:

\[
    r = \sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2}
\]

For \( r > 0 \) in vector form:

\[
    \mathbf{r} = [x - x_0, y - y_0, z - z_0] = (x - x_0)\mathbf{i} + (y - y_0)\mathbf{j} + (z - z_0)\mathbf{k}
\]
Therefore;

$$|r| = r$$

and \((-1/r)r\) is a unit vector in the direction of \(p\). The minus sign indicates that \(p\) is directed from \(P\) to \(P_0\). Thus,

$$p = |p| \left( -\frac{1}{r}r \right) = -\frac{c}{r^3} \mathbf{r} = -\frac{c}{r^3} (x - x_0) \mathbf{i} - \frac{c}{r^3} (y - y_0) \mathbf{j} - \frac{c}{r^3} (z - z_0) \mathbf{k}$$
Example 2:
From the former example, by the Newton’s Law of Gravitation, the force of attraction between 2 particles is given as:

\[ \mathbf{p} = -\frac{c}{r^3} \mathbf{r} = -c \left( \frac{x-x_0}{r^3} \mathbf{i} + \frac{y-y_0}{r^3} \mathbf{j} + \frac{z-z_0}{r^3} \mathbf{k} \right) \]

where \( r \) is a distance between two particles \( P_0 \) and \( P \) of the given coordinates. Thus,

\[ r = \sqrt{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2} \]
The important observation now is

\[
\frac{\partial}{\partial x} \left( \frac{1}{r} \right) = \frac{-2(x - x_0)}{2[(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2]^{3/2}} = -\frac{x - x_0}{r^3}
\]

Similarly;

\[
\frac{\partial}{\partial y} \left( \frac{1}{r} \right) = -\frac{y - y_0}{r^3}
\]

and

\[
\frac{\partial}{\partial z} \left( \frac{1}{r} \right) = -\frac{z - z_0}{r^3}
\]
From here, it is observed that $p$ is the gradient of the scalar function;

$$f(x, y, z) = \frac{c}{r}$$

and $f$ is a potential of that gravitational field. Applying the Laplace Equation of the form;

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = 0$$
Introduction and Concepts

Applying this to the unit vector, gives for the individual component:

\[
\frac{\partial^2}{\partial x^2} \left( \frac{1}{r} \right) = -\frac{1}{r^3} + \frac{3(x-x_0)^2}{r^5}
\]

\[
\frac{\partial^2}{\partial y^2} \left( \frac{1}{r} \right) = -\frac{1}{r^3} + \frac{3(y-y_0)^2}{r^5}
\]

\[
\frac{\partial^2}{\partial z^2} \left( \frac{1}{r} \right) = -\frac{1}{r^3} + \frac{3(z-z_0)^2}{r^5}
\]
Combining the 3 gives;

\[
\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \frac{c}{r} = 0
\]

or it can be written in the form of;

\[
\nabla^2 f = 0
\]

which is normally termed as the **Laplacian operator** of a function.
Example 3:
From Example 2, it is known that the gravitational force $\mathbf{p}$ is the gradient of the scalar function $f(x, y, z) = \frac{c}{r}$ which satisfies Laplace’s equation $\nabla^2 f = 0$. Therefore,

$$\text{div } \mathbf{p} = 0$$

for $r > 0$.  

Example 4:
Consider a motion of a fluid in a region $R$ having no sources and sinks in $R$ (no points at which the fluid is produced or disappeared). Assuming that the fluid is compressible and it flows through a small rectangular box $W$ of dimension $\Delta x$, $\Delta y$ and $\Delta z$ with edges parallel to the coordinate axes. $W$ has a volume of $\Delta V = \Delta x \Delta y \Delta z$. Let $\mathbf{v}$ is the velocity vector of the form given by:

$$\mathbf{v} = [v_1, v_2, v_3] = v_1 \mathbf{i} + v_2 \mathbf{j} + v_3 \mathbf{k}$$
Setting

\[ \mathbf{u} = \rho \mathbf{v} = [u_1, u_2, u_3] = u_1 \mathbf{i} + u_2 \mathbf{j} + u_3 \mathbf{k} \]

where \( \rho \) is the density of the fluid. Consider the flow of fluid out of the box \( W \) is through the left face whose area is \( \Delta x \Delta z \) and the components \( v_1 \) and \( v_3 \) are parallel to that face and contribute nothing to that flow. Thus, the mass of fluid entering through that face during a short time interval \( \Delta t \) is approx. given by;

\[ (\rho v_2)_y \Delta x \Delta z \Delta t = (u_2)_y \Delta x \Delta z \Delta t \]
And the mass of fluid leaving the opposite face of the box \( W \), during the same time interval is approx. given by:

\[
(u_2)_{y+\Delta y} \Delta x \Delta z \Delta t
\]

Therefore, the difference is in the form of:

\[
\Delta u_2 \Delta x \Delta z \Delta t = \frac{\Delta u_2}{\Delta y} \Delta V \Delta t
\]

where

\[
\Delta u_2 = (u_2)_{y+\Delta y} - (u_2)_y
\]
Two other pairs in $x$ and $z$ directions are taken and combined in the form given by;

$$
\left( \frac{\Delta u_1}{\Delta x} + \frac{\Delta u_2}{\Delta y} + \frac{\Delta u_3}{\Delta z} \right) \Delta V \Delta t
$$

The loss of mass in $W$ is caused by the rate of change of the density and therefore equals to;

$$
- \frac{\partial \rho}{\partial t} \Delta V \Delta t
$$
Equating both equations gives;

\[
\left( \frac{\Delta u_1}{\Delta x} + \frac{\Delta u_2}{\Delta y} + \frac{\Delta u_3}{\Delta z} \right) \Delta V \Delta t = -\frac{\partial \rho}{\partial t} \Delta V \Delta t
\]

Diving the above equation by \( \Delta V \Delta t \) and let \( \Delta x, \Delta y, \Delta z \) and \( \Delta t \) approaching 0 leads to;

\[
\left( \frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial y} + \frac{\partial u_3}{\partial z} \right) = -\frac{\partial \rho}{\partial t}
\]
Or in its simplified form:

\[ \text{div } \mathbf{u} = -\frac{\partial \rho}{\partial t} \]

or

\[ \text{div}(\rho \mathbf{v}) = -\frac{\partial \rho}{\partial t} \]

which consequently becomes;

\[ \frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{v}) = 0 \]

which is the condition for the conservation of mass or the continuity equation of a compressible fluid flow!
If the flow is **steady**, or it is independent of time, thus:

\[
\frac{\partial \rho}{\partial t} = 0
\]

and therefore the continuity equation reduces into

\[
\text{div}(\rho \mathbf{v}) = 0
\]

If the density \( \rho \) is constant, which means the fluid is incompressible, therefore the continuity equation becomes;

\[
\text{div} \ \mathbf{v} = 0
\]
Consider a parallel plates with area $A$ separated by distance $Y$ with a type of fluid:

- The system is initially at rest
- At time $t = 0$, the lower plate is set in motion in the positive $x$ direction at a constant velocity $V$.
- As time proceeds, the fluid gains momentum and the linear steady-state velocity is established.
- At steady motion, a constant force, $F$ is required to maintain the motion of the lower plate and this can be expressed as:

$$\frac{F}{A} = \mu \frac{V}{Y}$$
Viscosity and the Mechanisms of Momentum Transport

\[ v_x(y,t) \]

\[ v_x(y) \]

\( t < 0 \) Fluid initially at rest

\( t = 0 \) Lower plate set in motion

Small \( t \) Velocity build up in unsteady flow

Large \( t \) Final velocity distribution in steady flow
Consider a parallel plates with area $A$ separated by distance $Y$ with a type of fluid;

1. Force in the direction of $x$ perpendicular to the $y$ direction given by $F/A$ is replaced by $\tau_{yx}$.

2. The term $V/Y$ is replaced by $-dv_x/dy$ and therefore the equation becomes;

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

This means that the shearing force per unit area is proportional to the negative of the velocity gradient i.e. Newton’s Law of Viscosity.
Similarly, let the angle between the fixed plate and the moving boundary $\delta \gamma$ and the distance from the origin is $\delta x$.

Therefore,

$$\tan \delta \gamma = \frac{\delta x}{Y}$$

for a very small angle,

$$\frac{\delta x}{Y} = \delta \gamma$$
But

\[ \delta x = V \delta t \]

thus,

\[ \delta \gamma = \frac{V \delta t}{Y} \]

Taking limit on the above terms;

\[
\lim_{\delta t \to 0} \frac{\delta \gamma}{\delta t} = \frac{V}{Y} = \frac{dv}{dy}
\]
Hence;

\[
\frac{\delta \gamma}{\delta t} \sim \frac{dv}{dy}
\]

But

\[
\dot{\gamma} \sim \tau
\]

Thus,

\[
\tau \sim \frac{dv}{dy}
\]
Viscosity and the Mechanisms of Momentum Transport

Which then becomes

\[ \tau = -\mu \frac{dv}{dy} \]

with \( \mu \) as the proportionality constant.

The minus sign represents the force exerted by the fluid of the lesser \( Y \) on the fluid of greater \( Y \).
Viscosity and the Mechanisms of Momentum Transport

\[ \tau \sim \frac{d\gamma}{dt} \]

- **Shear thinning**
- **Newtonian**
- **Shear thickening**
Viscosity and the Mechanisms of Momentum Transport

Generalisation of Newton’s Law of Viscosity.

- Consider a fluid moving in 3-dimensional space with respect to time $t$.

- Therefore, the velocity components are given as follows:

$$v_x = v_x(x, y, z, t) \quad v_y = v_y(x, y, z, t) \quad v_z = v_z(x, y, z, t)$$

- In the given situation, there will be 9 stress components, $\tau_{ij}$. 
Viscosity and the Mechanisms of Momentum Transport

Based on the given diagram:

1. The pressure force-always perpendicular to the exposed surface.

2. Thus, the force per unit area on the shaded surface will be a vector $p\delta_x$ (pressure multiplied by the unit vector $\delta_x$ in the $x$ direction)

3. Same goes to the $y$ and $z$ directions.
Viscosity and the Mechanisms of Momentum Transport

The velocity gradients within the fluid are neither perpendicular to the surface element nor parallel to it, but rather at some angle to the surface.

The force per unit area, $\tau_x$ exerted on the shaded area with components ($\tau_{xx}$, $\tau_{xy}$ and $\tau_{xz}$).

This can be conveniently represented by standard symbols which include both types of stresses (pressure and viscous stresses);

$$\pi_{ij} = p\delta_{ij} + \tau_{ij}$$

where $i$ and $j$ may be $x$, $y$ or $z$. 
Viscosity and the Mechanisms of Momentum Transport

Here, $\delta_{ij}$ is the Kronecker delta, which is 1 if $i = j$ and zero if $i \neq j$.

The term $\pi_{ij}$ can be defined as:

- force in the $j$ direction on a unit area perpendicular to the $i$ direction, where it is understood that the fluid in the region of lesser $x_i$ is exerting the force on the fluid of greater $x_i$.
- flux of $j$-momentum in the positive $i$ direction – that is, from the region of lesser $x_i$ to that of greater $x_i$. 
Viscosity and the Mechanisms of Momentum Transport

Summary of the components of the molecular stress tensor.

<table>
<thead>
<tr>
<th>Dir.</th>
<th>Vector force</th>
<th>Components of forces</th>
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</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>x-component</td>
</tr>
<tr>
<td>$x$</td>
<td>$\pi_x = p\delta_x + \tau_x$</td>
<td>$\pi_{xx} = p + \tau_{xx}$</td>
</tr>
<tr>
<td>$y$</td>
<td>$\pi_y = p\delta_y + \tau_y$</td>
<td>$\pi_{yx} = \tau_{yx}$</td>
</tr>
<tr>
<td>$z$</td>
<td>$\pi_z = p\delta_z + \tau_z$</td>
<td>$\pi_{zx} = \tau_{zx}$</td>
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