

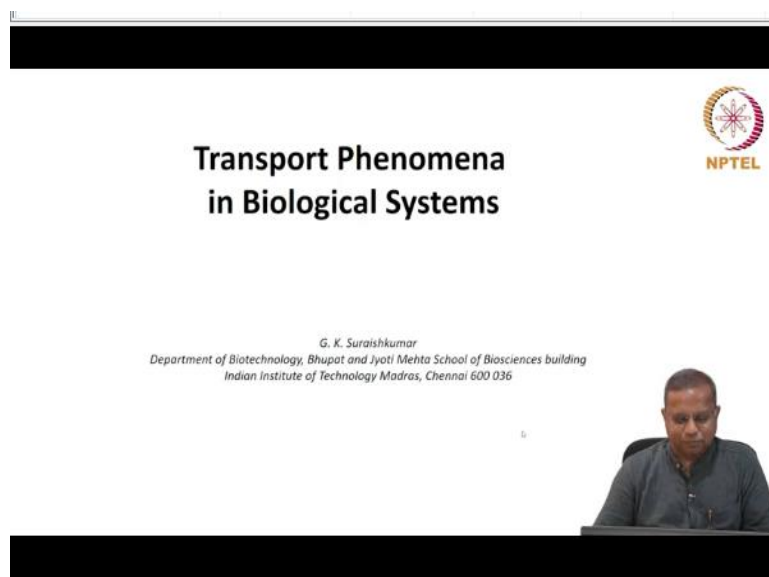
Transport Phenomena in Biological Systems
Prof. G. K. Suraishkumar
Department of Biotechnology Bhupat and Jyoti Mehta School of Biosciences Building
Indian Institute of Technology-Madras

Lecture-78
Course Review-Part 1

Welcome, in the next few lectures, this lecture and then probably one or two more, we would review the entire course, this is a heavy course and therefore we are going to take a time reviewing it, you would be able to look at things and perspective, you would be able to revise the concepts, cement some of those concepts that are still eluding you and so on and so forth. So, that your overall preparation becomes that much better.

So it is nice to have all the review in one later on. If you want to refer to this course you can start with the review. There you have everything in a form that is there you have already gone through the effort in arriving at these various things. And based on your need, you can go to the specific lectures which are much more detailed okay.

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So, let us begin with the place where we began. I told you initially where this course fits in because you need to understand that to appreciate the course, a little better.


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Engineering curricula

Engineering undergraduates in respective disciplines are given the knowledge and are helped to understand the same toward analysis and design of the appropriate systems, after graduation.

For example, Mechanical Engineers are expected to analyze, design, and operate Mechanical systems, Electrical engineers are expected to do the same for Electrical systems, Chemical Engineers for Chemical systems, and so on.

Similarly, Biological Engineering graduates are expected to analyze, design, and operate biological systems. For the above, they need to have an appropriate understanding based on the suitable knowledge provided to them.

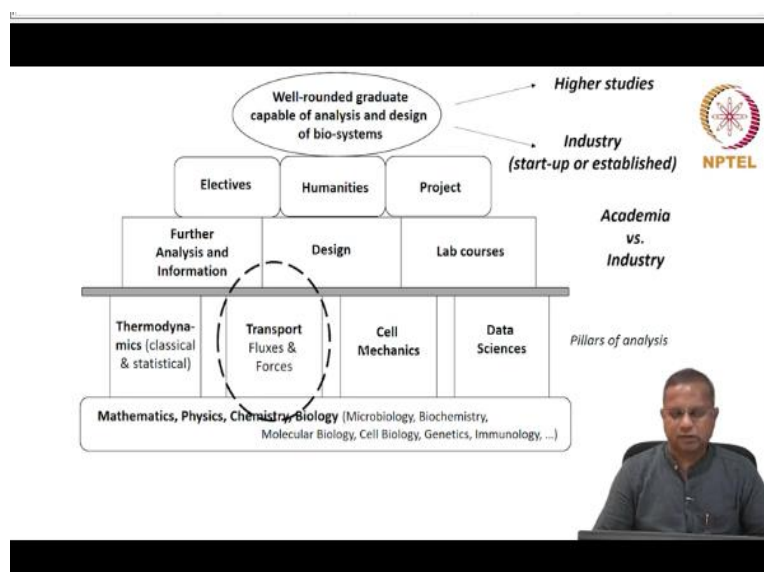




So, we looked at engineering curricula in general and we said that engineers are expected to analyze design and operate appropriate systems. Mechanical Engineers are expected to analyze and design and operate mechanical systems. Electrical engineers are expected to do the same for electrical systems, chemical engineers are chemical systems and so on and so forth. Similarly, biological engineering graduates are expected to analyze design and operate biological systems.

That is what engineering is all about. For the above they need to have an appropriate understanding based on these suitable knowledge that is provided to them was what the bottom line was.

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So, the curriculum is typically set up like this we have a base in mathematics, physics, chemistry and biology. We provide the base predominantly for biology, even the initial information that many students will not have. Mathematics, physics and chemistry they come in with some preparation and then that level is raised through the first year engineering courses.

And first year maths, physics, chemistry courses in engineering, then you have pillars of analysis, one of the important pillars is thermodynamics both the classical and statistical aspects for biological systems. Transport, this course fluxes and forces, cell mechanics, the courses that give you a course that looks at the mechanical aspects of cells and data sciences, the way of looking at large data sets to make appropriate sense.

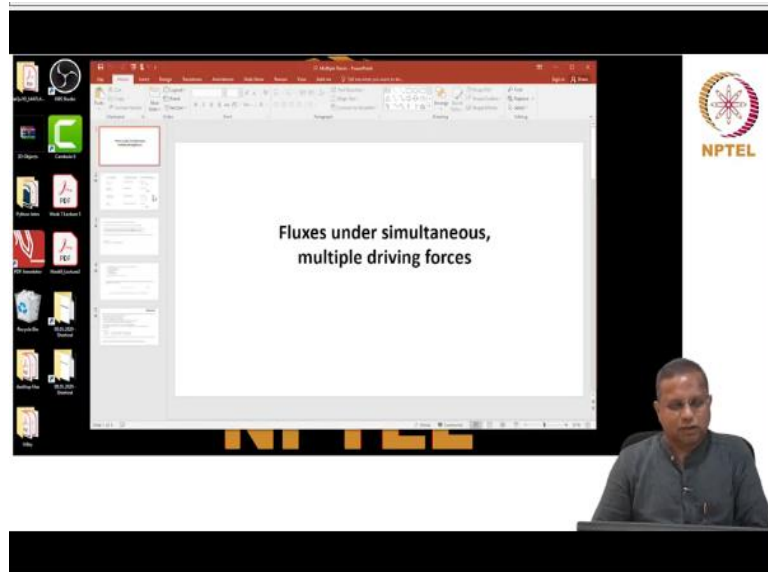
All these are pillars of analysis of the basic information that is provided. So, there are courses for all these aspects and on top of this we have courses. So, further analysis as well as information, specific information, design, lab courses, which helps students develop a lot of necessary skills. Then you have electives which could be short term electives are topical or could be topical.

There is a certain interest in a certain topic at a certain time in the world. So, there is a course that is given on that mostly information and some analysis and so on. They could also be courses that built on these, which are electives. Electives this means the person has a choice to do them, which are not the essential aspects of the curriculum, but build on to the curriculum, add on to the value of the person.

Then, of course, you need humanities courses for a well rounded development of the graduate, you typically have a project to all these together, go towards making a well rounded graduate, capable of analysis and design of biosystems. Then the graduate either goes, I mean goes out into the real world and either into the industry, either a start up or an established industry, or goes for higher studies that will lead to academia or a industry.

This is the place for this course. And therefore, the importance, it is one of the pillars of analysis, important foundation for the entire curriculum and therefore it is important. We have already seen this.

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And then this is a textbook and so on, so forth. I think that is good enough for the introductory aspect of this course.

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Thus far,

Flux of quantity	Primary driving force	A constitutive equation
Mass (conserved)	concentration gradient	Fick's 1 law $\vec{J}_i = -D_i \frac{dc_i}{dx}$
Momentum (conserved)	velocity gradient	Newton's law $\tau_{yx} = -\mu \left(\frac{dv_x}{dy} \right)$
Thermal Energy (not conserved)	temperature gradient	Fourier's law $q_x = -k \frac{dT}{dx}$
Charge (conserved)	electrical potential gradient	Ohm's law $\vec{J} = -k_e \frac{\partial V}{\partial x}$

The image shows a table with three columns: "Flux of quantity", "Primary driving force", and "A constitutive equation". It lists four rows of physical quantities: Mass (conserved), Momentum (conserved), Thermal Energy (not conserved), and Charge (conserved). Each row provides the primary driving force and the corresponding constitutive equation. The NPTEL logo is in the top right, and a small inset video shows a man in a grey shirt speaking.

Now, let me switch to this aspect which in a nutshell puts the various perspectives together, okay. If you look at, we had essentially looked at the fluxes of conserved quantities which has mass, momentum, energy and charge okay. These are the 4 conserved quantities that we looked at in this course. If you look at the flux of that particular conserved quantity, the primary driving force for that quantity in this column.

And a constitutive equation, which is obeyed by a wide variety of substances may not be all but a wide variety of substances here, then, if you look at mass which is conserved, the concentration gradient is the primary driving force and Fick's first law gives you an example

of a constitutive equation. The molar flux is directly proportional to the negative of the concentration gradient and the constant of proportionality is a diffuser.

Then if you look at momentum flux, momentum is also conserved. Velocity gradient is the primary driving force and Newton's law of viscosity, which is τ_{yx} , the shear stress τ_{yx} equals $-\mu \frac{dv_x}{dy}$. The momentum flux is proportional to the velocity gradient, the negative of the velocity gradient and the constant of proportionality is your viscosity. Then we looked at thermal energy which is not conserved.

We looked at energy conservation as a whole then we kind of picked out or backed out thermal energy from this because thermal energy is of importance to us in design an operation. Temperature gradient is the primary driving force in this case and Fourier's law q_x , heat flux is directly proportional to the negative of the temperature gradient with the constant of proportionality being the heat conductivity.

You see all these forms being the same, all these ideas being the same and so on. One more charge which is of course a conserved quantity, the primary driving force is the electrical potential gradient and the Ohm's law, which is sorry the electrical charge flux being proportional to the negative of the electrical potential gradient and the constant of proportionality being the electrical conductivity k_e .

The potential gradient divided by $1/k_e$ which is the resistance is your current and so on so forth. This is of course is flux, this is written in terms of fluxes to be consistent with our other representations and in this course. This gives you in a nutshell, what are we looked at in a majority of the course, where we looked only at the primary driving force causing the appropriate books. And then the last chapter was something else. Now let me go back to details. In this lecture, I look at the details of mass conservation.

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The slide is titled "Conserved Quantities" and lists "Conserved physical quantities" as Mass, Momentum, Energy, and Charge. It states that for a conserved quantity, we can confidently say/write LHS = RHS, say in a process. It then says we would consider the fluxes of conserved quantities and provides the formula: Flux of a quantity = (Quantity moved / Time) * (1 / Area perpendicular to the direction of movement). The NPTEL logo is in the top right corner.

And mass flux is mass conservation is an important principle.

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The slide discusses mass conservation. It states "We all know 'Mass can neither be created nor destroyed' from high school physics". It then says "Mass is conserved" and lists two conditions: "- if we are not dealing with nuclear reactions (mass to energy conversion)" and "- if we are not travelling at close to light speeds (mass dilation)". It concludes by saying "Let us first review some useful applications of the mass conservation principle and also extend it" and "Before that, let us review the more fundamental, 'rate concept'". The NPTEL logo is in the top right corner.

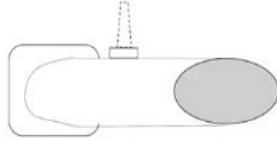
We saw the need for rates. That is where we began actually at the very, very beginning. When because engineering quantities look at rates, okay. And so we needed to write or we needed to express the mass conservation principle, mass can neither be created nor destroyed in terms of rates relevant to a process and that is the way it was going to become useful. Also, I need to mention that of course, mass is conserved as long as we are not dealing with nuclear reactions, where mass to energy conversion can take place.

Or we are not travelling at speeds close to that applied in these conditions. When you travel at speeds close to that of light, you get mass dilation. So we are not looking at that affects in the



mass conservation. So, as long as you do not get into these masses conserved for all terrestrial aspects except for nuclear reactions and then they should be fine.

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Let us say that we are filling a water tank of volume, $V = 12,000 \text{ L}$



mass, $m = ?$ *pause* 12,000 Kg





So, we had reviewed the mass conservation principle.

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r_{in} , Input rate (Kg s^{-1})	t , time (s)
10	1200 (20 min)
20	600 (10 min)
50	240 (4 min)

If we know the **rate** of water input, r_{in} , $t = m / r_{in}$



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Suppose, there is a hole in the tanker, which oozes water at a rate of 5 Kg s^{-1} , how long would it take to fill the tank?

...

pause

$$r_{\text{net}} = r_{\text{in}} - r_{\text{out}} = 20 - 5 = 15 \text{ Kg s}^{-1}$$

$$t = m / r_{\text{net}} = 12000 / 15 = 800 \text{ s (or, 13.3 min)}$$



We looked at the need for it and so on.

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Now, suppose, that in addition to the leak, there is some mechanism inside the tank itself that is generating water at say 1 Kg s^{-1} and some other reaction in which water is used up inside the tank, at 0.25 Kg s^{-1} , all of which **simultaneously occur**, how long would it take to fill the tank?



pause

$$r_{\text{net}} = r_{\text{in}} - r_{\text{out}} + r_{\text{gen}} - r_{\text{consump}} = 20 - 5 + 1 - 0.25 = 15.75 \text{ Kg s}^{-1}$$

This is the rate at which water gets **accumulated** inside the tank, the rate of change of water mass with time in the tank (system)

$$t = m / r_{\text{net}} = 12000 / 15.75 = 761.9 \text{ s (or, 12.7 min)}$$

***Rate is a fundamental (in terms of usefulness) parameter.
You need to start thinking in terms of rates rather than amounts
any mass or volume, as you did in school***



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Mass balance: important principle



Based on the law of conservation of mass

Total mass is a constant
(as long as we don't deal with nuclear reactions, or
travel at speeds close to that of light)

If we follow the mass of a species, only the following
can happen to the species:



- Species is input into the system (rate: r_i)
- Species is output from the system (rate: r_o)
- Species is generated in the system (rate: r_g)



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$$\text{net rate} = r_i - r_o + r_g - r_c$$



net rate = rate at which the species mass gets
accumulated in the system, $\frac{dm}{dt}$

$$r_i - r_o + r_g - r_c = \frac{d(m)}{dt}$$

This is a useful form of the material balance principle,
that can be directly applied to processes



And then we got a useful form of the mass conservation equation, input rate in a mass rate minus the output rate plus the generation rate minus the consumption rate equals the accumulation rate okay. This in fact can generally be used for any conserved quantity, here we had use it for mass, then we use it for momentum, then we use it for charge and then we use it for energy and then for charge, okay.

So, this is general common sense there is nothing else than that can happen to any species. There can be when you focus on a system and you focus on a species in the system you do a balances over the system, there can be only an input rate and output rate a generation rate and a consumption rate and the algebraic sum of those leads to the accumulation rate. It is written in this form to be directly in a useful form for the various analyses.


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Reflection/Practice point

Application to macroscopic systems

A humidifier is fed with dry air (with no water vapour; it is removed during the processing of air to avoid contamination of the bioreactor) and clean liquid water. *Why use a humidifier?*

The liquid water flow rate is 18 cc min^{-1} . If 5 mole% of oxygen are needed in the output stream of the humidifier for supply to the bioreactor, let us determine the molar rate at which air should be supplied to the humidifier, when it operates at steady-state.






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Problem solving





So, we had looked at the application to macro system which is a review.

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Problem solving is a higher level **skill**



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Closed-ended problem solving



0. Get a feel of the situation by reading it a few times
1. What is needed?
2. What is given/known?
3. How do we connect the needs with the givens/knowns?

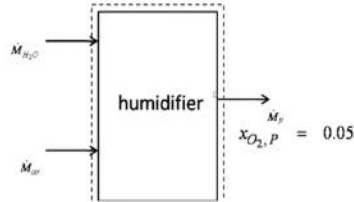
Any principles that we can rely on?



Then we looked at some principles of problem solving okay. Essentially I get a feel for the situation by reading it a few times. This is for close ended problem solving that is and then ask the question what is needed, what is given or known you could do that in any order, and then, how to connect the needs with the givens or knowns. This in general is the algorithm for getting or solving problems which are closed ended.

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A humidifier is fed with dry air (with no water vapour; it is removed during the processing of air to avoid contamination of the bioreactor) and clean liquid water. *Why use a humidifier?*
 The liquid water flow rate is 18 cc min^{-1} . If 5 mole% of oxygen are needed in the output stream of the humidifier for supply to the bioreactor, let us determine the molar rate at which air should be supplied to the humidifier, when it operates at steady-state.



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0. Get a feel of the situation by reading it a few times



1. What is needed? Molar rate of air at the outlet of the humidifier

2. What is given/known? Flow rates and compositions of some streams

3. How do we connect the needs with the givens/knowns?

Any principles that we can rely on? Material balance

*It is recommended to do the above, explicitly while solving closed-ended problems
 We would do it mostly implicitly*






So, this was the application to a macroscopic system, which was a review.

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Let us work with moles because of the requirements of the problem.
 Mole = mass/molecular mass, and if there is no change in the species, say due to a reaction during the process, the mole balances on individual species are as good as the mass balances.
 When in doubt, balance masses to be sure.

Dry air is made of 21% oxygen and 79% nitrogen by volume or mole (the minor components of air are ignored for this problem).
 Thus, the molar flow rates of oxygen and nitrogen in the air stream can be written as:

$$\dot{M}_{O_2, air} = 0.21 \dot{M}_{air} \quad \text{Eq. 1.3. - 1}$$







And then we applied it to a microscopic system. Maybe not spend too much here, the microscopic system, I think is here or here. Yeah, it is here.

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Application to microscopic systems: A biological cell

We know from our basic biology courses that thousands of reactions occur in simultaneously occurring reaction networks in a cell
 They are essential for normal cell function
 The bio-products are also made as a results of such reaction networks

Metabolic Flux Analysis (MFA) is a method of analysis of reaction networks
 It has been successfully used to modify cells toward significantly improved product yields

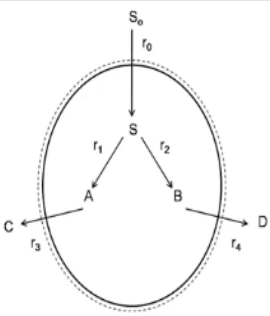
So, this is application to a microscopic system or a biological cell, where we looked at the reaction network in the cell and looked at the essence of metabolic flux analysis.

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Let us consider a few reactions that occur in the cell

The rates of the individual steps, r_0 , r_1 , r_2 , r_3 , and r_4 (mmole per second), or mmole (g cell)⁻¹ s⁻¹

Historically, the above **rates** are called metabolic 'fluxes'. This 'flux' is different from the normal meaning of the term in this course

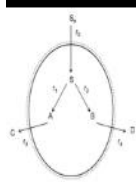


For the intracellular metabolites (S, A, B), we will consider the intracellular space of the cell as our system




We considered a framework. We wrote the balances for each of these components in the framework. Okay, in the reaction framework. The trick that we used was that for the intracellular metabolites, we would use the inside of the cell as system for extra cell metabolites were used the outside of the cell as a system, the thing that we focus on.

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$$r_i - r_o + r_g - r_c = \frac{d(m)}{dt}$$


Balance on S_0	$-r_0$				$= \frac{dS_0}{dt}$
Balance on S	r_0	$-r_1$	$-r_2$		$= \frac{dS}{dt}$
Balance on A		r_1		$-r_3$	$= \frac{dA}{dt}$
Balance on B			r_2	$-r_4$	$= \frac{dB}{dt}$
Balance on C				r_3	$= \frac{dC}{dt}$
Balance on D				r_4	$= \frac{dD}{dt}$



Then when we wrote the balances.

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These balance equations can be written in a compact form, as follows:




$$\begin{bmatrix} -1 & 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} r_0 \\ r_1 \\ r_2 \\ r_3 \\ r_4 \end{bmatrix} = \frac{d}{dt} \begin{bmatrix} S_0 \\ S \\ A \\ B \\ C \\ D \end{bmatrix} \quad \text{Eq. 1.2-9}$$

or

$$\tilde{S} \cdot \tilde{r} = \frac{d}{dt} \tilde{x} \quad \text{Eq. 1.2-10}$$

Eq. 1.2-10 is used to quantify metabolic fluxes for further MFA.

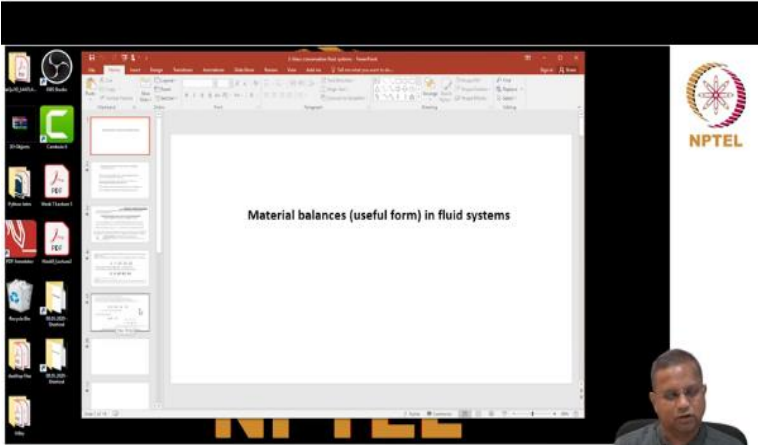

- \tilde{S} = stoichiometric matrix
- \tilde{r} = reaction rate vector
- \tilde{x} = state vector (vector of state variables)



We could write it of the form that can be transferred to a compact matrix form, the stoichiometric matrix, the rate vector and the vector of state variables the derivative of that is what the balance comes down to and this is very useful in different situations. You need of course, much more specifics to be able to make appropriate use of this formulation, okay. So, $S \cdot r = \frac{dx}{dt}$, S matrix, r matrix or r vector and the derivative of this state variable vector.

So, stoichiometric matrix, reaction rate vector and these state vector, vector of state variables. So, this is what we had seen. And then we started looking at fluxes, we defined what a flux was.

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Before that we looked at mass conservation. So, I need to mention this.

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We considered a fluid flow situation.

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Review of needed derivatives

Let us ensure that we are comfortable with the need for a mathematical approach and the needed derivatives.

A mathematical approach makes aspects more generally applicable and thus, significantly increases our confidence in its use

To review the derivatives, let us consider studying the effect of ocean currents on fish concentration in the ocean, with a sonar device for fish counts and a motor boat

The fish concentration, $c = f(x, y, z, t)$ i.e. function of (can vary with) space and time

If we drop the effective anchors of the motor boat, and count the fish, the count will provide the variation of c w.r.t. time alone, because we are doing it at a fixed location, i.e. fixed x, y, z

$\left(\frac{\partial c}{\partial t}\right)_{x,y,z}$ i.e. **partial derivative** of c with respect to t , at constant x, y, z
Usually x, y, z are not explicitly shown as constants in the partial derivative, except when required to avoid confusion

And then we said that we needed, we looked at derivatives that we needed and the review mode, partially derivative.

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Next, let us raise the anchor, start the engine and move about in the ocean, and count fish with our device.

The time rate of change of c will give (easy to see by applying the chain rule to $c = f(t, x, y, z)$)



$$\frac{dc}{dt} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial c}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial c}{\partial z} \frac{\partial z}{\partial t}$$

$c = f(t, x, y, z)$, but $x = f(t)$, $y = f(t)$, $z = f(t)$, i.e. only functions of t .

Thus we can replace those partial derivatives with t by total derivatives

$$\frac{dc}{dt} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} \frac{dx}{dt} + \frac{\partial c}{\partial y} \frac{dy}{dt} + \frac{\partial c}{\partial z} \frac{dz}{dt}$$

$\frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt}$ are components of the boat velocity
 $\frac{\partial c}{\partial x}, \frac{\partial c}{\partial y}, \frac{\partial c}{\partial z}$ are components of the concentration changes with respect to the boat's position at a certain time

A total derivative and then we also looked at the substantial derivative which you may be familiar with or you may have picked up as a part of this course, okay.

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Let us say, we shut off the engines, but do not drop anchor

We would move about with the velocity of the current, \vec{v} (local velocity)

The change in fish concentration with time will depend on the local velocity, \vec{v}

Such a derivative is called 'time derivative following the motion' or "substantial derivative"

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + v_x \frac{\partial c}{\partial x} + v_y \frac{\partial c}{\partial y} + v_z \frac{\partial c}{\partial z}$$

v_x, v_y, v_z are the components of the local velocity \vec{v}



More compactly, in vector notation:

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + (\vec{v} \cdot \vec{\nabla} c)$$

$$\vec{v} = i v_1 + j v_2 + k v_3$$

$$\vec{\nabla} = i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z}$$

The $i, j,$ and k are the unit vectors in the x, y and z directions, respectively

So, these are the 3 derivatives that would be used in this course, very useful derivatives and the compact notation that we can use, this is the equation of continuity for a single component system or the total mass taken in terms of substantial derivative here. That is what we had come to.

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Useful form of material balance in a flow (fluid) system
Useful form: in terms of measurable/relevant variables



Equation of continuity

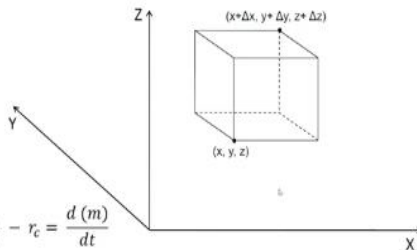
Let us first consider a single component (or total mass)



Before we got into the flux, you still follow the middle. Yeah, I had already given you a flavour of how things would be, we derive equations with a reasonably gentle have those tables, just refer to the tables, choose the appropriate equation, cancel out the relevant terms and go forward okay.

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Let us choose a right handed Cartesian co-ordinate system
 Let us choose a fixed volume element in space through which the fluid flows
 Volume of the element, $\Delta V = \Delta x \Delta y \Delta z$



$$r_i - r_o + r_g - r_c = \frac{d(m)}{dt}$$

If a single component system or total mass is considered, there will be no generation or consumption. Thus, the balance becomes

$$r_i - r_o = \frac{d(m)}{dt}$$




So, I have shown you the equation of continuity, derive the equation of continuity, take in the rectangular Cartesian coordinate system.

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Let us express the balance in terms of measurable/relevant variables.


This is a 3-D flow. We need to consider the contributions from all directions. Let us do them one by one.

Recall ρ (kg m^{-3}) $\times v$ (m s^{-1}) = mass flux ρv ($\text{kg m}^{-2} \text{s}^{-1}$). And, rate = (flux) \times (area)



Rate of mass in through the face at x	$= (\rho v_x) _x \Delta y \Delta z$
Rate of mass out through the face at $x + \Delta x$	$= (\rho v_x) _{x+\Delta x} \Delta y \Delta z$
Rate of mass in through the face at y	$= (\rho v_y) _y \Delta x \Delta z$
Rate of mass out through the face at $y + \Delta y$	$= (\rho v_y) _{y+\Delta y} \Delta x \Delta z$
Rate of mass in through the face at z	$= (\rho v_z) _z \Delta x \Delta y$
Rate of mass in through the face at $z + \Delta z$	$= (\rho v_z) _{z+\Delta z} \Delta x \Delta y$
Rate of mass accumulation within the volume element	$= \frac{\partial(\rho V)}{\partial t} = \frac{\partial(\rho \Delta x \Delta y \Delta z)}{\partial t} = \Delta x \Delta y \Delta z \frac{\partial \rho}{\partial t}$

Substituting the above in 1.4.3-2, i.e.



And extended that Cartesian.

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$$\Delta x \Delta y \Delta z \frac{\partial \rho}{\partial t} = \Delta y \Delta z \{(\rho v_x)|_x - (\rho v_x)|_{x+\Delta x}\} + \Delta x \Delta z \{(\rho v_y)|_y - (\rho v_y)|_{y+\Delta y}\} + \Delta x \Delta y \{(\rho v_z)|_z - (\rho v_z)|_{z+\Delta z}\} \quad \text{Eq. 1.4.3-3}$$


Divide throughout by $\Delta x \Delta y \Delta z$ **pause**

$$\frac{\partial \rho}{\partial t} = \frac{1}{\Delta x} \{(\rho v_x)|_x - (\rho v_x)|_{x+\Delta x}\} + \frac{1}{\Delta y} \{(\rho v_y)|_y - (\rho v_y)|_{y+\Delta y}\} + \frac{1}{\Delta z} \{(\rho v_z)|_z - (\rho v_z)|_{z+\Delta z}\}$$

When we impose the limit of an infinitesimal volume i.e. $\Delta x \rightarrow 0, \Delta y \rightarrow 0,$ and $\Delta z \rightarrow 0$ **pause**

$$\frac{\partial \rho}{\partial t} = - \left(\frac{\partial}{\partial x} \rho v_x + \frac{\partial}{\partial y} \rho v_y + \frac{\partial}{\partial z} \rho v_z \right) \quad \text{Eq. 1.4.3-4}$$

Vectorially, $\frac{\partial \rho}{\partial t} = -(\vec{\nabla} \cdot \rho \vec{v})$ Eq. 1.4.3-5 **Equation of continuity**



The equation of continuity to other coordinate systems.

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Let us re-consider Eq. 1.4.3.-4
$$\frac{\partial \rho}{\partial t} = - \left(\frac{\partial}{\partial x} \rho v_x + \frac{\partial}{\partial y} \rho v_y + \frac{\partial}{\partial z} \rho v_z \right)$$

Let us expand the RHS using chain rule

$$\frac{\partial \rho}{\partial t} = - \left[\rho \frac{\partial v_x}{\partial x} + v_x \frac{\partial \rho}{\partial x} + \rho \frac{\partial v_y}{\partial y} + v_y \frac{\partial \rho}{\partial y} + \rho \frac{\partial v_z}{\partial z} + v_z \frac{\partial \rho}{\partial z} \right]$$

Let us re-arrange the above as

$$\frac{\partial \rho}{\partial t} + v_x \frac{\partial \rho}{\partial x} + v_y \frac{\partial \rho}{\partial y} + v_z \frac{\partial \rho}{\partial z} = -\rho \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) \quad \text{Eq. 1.4.3.-6}$$

Using our definition of substantial derivative, we can write in vector notation:

$$\frac{D\rho}{Dt} = -\rho (\vec{v} \cdot \vec{\nabla})$$

Eq. 1.4.3.-7

Equation of continuity



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If the density is a constant (e.g. incompressible fluid, say liquid), it does not change w.r.t. time. Thus, the time derivatives of density can be set to 0.

The equation of continuity becomes

$$(\vec{v} \cdot \vec{\nabla}) = 0$$



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Reflection/Practice point



A design of a bioprocess device that is expected to handle a liquid presents the following flow description. Check whether the device is feasible

$$v_x = k_1(x^2 + y^2) \quad v_y = k_2(y^2 + z^2) \quad v_z = k_3(z^2 + x^2)$$



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Solution



The equation of continuity represents mass balance. Thus, it needs to be satisfied for any process to realistically exist.

Also, this is a liquid, which can be taken to be incompressible. Thus, for the given flow field, check whether

$$(\vec{v} \cdot \vec{v}) = 0$$

Or, whether $\left(\frac{\partial}{\partial x} v_x + \frac{\partial}{\partial y} v_y + \frac{\partial}{\partial z} v_z \right) = 0$ *pause*

Substituting the given flow field, the LHS gives $2k_1x + 2k_2y + 2k_3z$

$$= 2(k_1x + k_2y + k_3z)$$

Except at $k_1x + k_2y + k_3z = 0$ this is not zero

Since the validity is limited to a single plane, it does not seem to be suitable for design



Okay.

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In different coordinate systems



Rectangular coordinates:

$$\frac{\partial \rho}{\partial t} + \left(\frac{\partial(\rho v_x)}{\partial x} + \frac{\partial(\rho v_y)}{\partial y} + \frac{\partial(\rho v_z)}{\partial z} \right) = 0 \quad (A)$$

Cylindrical coordinates:

$$\frac{\partial \rho}{\partial t} + \left(\frac{1}{r} \frac{\partial(\rho r v_r)}{\partial r} + \frac{1}{r} \frac{\partial(\rho v_\theta)}{\partial \theta} + \frac{\partial(\rho v_z)}{\partial z} \right) = 0 \quad (B)$$

Spherical coordinates:

$$\frac{\partial \rho}{\partial t} + \left(\frac{1}{r^2} \frac{\partial(\rho r^2 v_r)}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(\rho v_\theta \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial(\rho v_\phi)}{\partial \phi} \right) = 0 \quad (C)$$

Appendix for transform



So, yeah, different coordinate systems. You have the rectangular coordinates here, which we derive. Then using the transformations in the appendix, it could go from the rectangle to the cylindrical coordinates from rectangle to the spherical coordinates. So, I would ask you to make a copy of this and keep it as a part of your notes to be used when there is a need okay. Then we started our mass flux.

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Mass Flux



So, flux of any quantity.



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As mentioned earlier,

$$\text{Flux of a quantity} = \left(\frac{\text{Quantity moved}}{\text{time}} \right) \left(\frac{1}{\text{Area perpendicular to the direction of movement}} \right)$$

$$\text{Mass flux} = \left(\frac{\text{Mass moved}}{\text{time}} \right) \left(\frac{1}{\text{Area perpendicular to the direction of movement}} \right)$$

In fluid systems,

$$\text{Density} \times \text{velocity} = \frac{\text{kg}}{\text{m}^3} \times \frac{\text{m}}{\text{s}} = \text{kg m}^{-2} \text{s}^{-1} \text{ is mass flux}$$





We have already seen was quantity moved per time, that was it is moving in this direction, per unit area that is perpendicular to the direction of motion. So, this was flux in this course, there were a few exceptions where the term flux was used differently, metabolic flux analysis was one such situation and the electric flux and magnetic flux from historical use of the term was a little different.

Apart from that, for this course, the flux meant this, quantity moved per time per unit area perpendicular to the direction of movement. Then, we said that the density times velocity is flux. We saw the various applications of this formulation, the basic formulation.

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Wide relevance

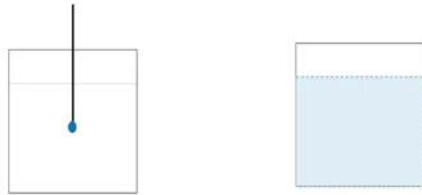
- Flux of substrates and products in bioreactors
- Flux of desirable substances in membrane filtration
- Glucose flux across the cell
- Product flux (e.g. ethanol) out, across the cell
- The transport of protein from the site of assembly to the site of function in the cell
- The mass flux of oxygen from the blood to the organ where the cells of the organ use it
- ...

The definitions of average.

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Let us consider this experiment:



Thermal motion



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What causes the flux?

A driving force

What is the driving force for mass flux?

A difference in concentration over a distance – concentration gradient

Strictly speaking, it is the chemical potential gradient, but for mass flux within the same phase, concentration gradient is sufficient

The concentration difference is 'primarily' or firstly linked to the mass flux

Many driving forces can cause much higher mass flux (e.g. stirring the beaker with ink)
We will see this in the last chapter – multiple driving forces causing the same flux



This is diffusion of course.

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Average velocities



Let us consider a multi-component mixture with many species (components)

Let \vec{v}_i be the velocity of i^{th} species with respect to stationary co-ordinates axes

The mass average velocity for a multi-species mixture with n species can be written as:

$$\vec{v} = \frac{\sum_{i=1}^n \rho_i \vec{v}_i}{\sum_{i=1}^n \rho_i} \quad \text{Eq. 2.1.1.-1}$$

Note: 'species' are not molecules

Species: A group of molecules of the same species i in a tiny volume element, take the sum of individual velocities of molecules of species i and divide by the number of such molecules in that tiny volume element.

Similarly, a molar average velocity \vec{v}^* is defined as:

$$\vec{v}^* = \frac{\sum_{i=1}^n c_i \vec{v}_i}{\sum_{i=1}^n c_i} \quad \text{Eq. 2.1.1.-2}$$



$$\vec{v} = \frac{\sum_{i=1}^n \rho_i \vec{v}_i}{\sum_{i=1}^n \rho_i} \quad (2.1.1-1)$$

where ρ_i is the density of the i^{th} species.

$$\vec{v}^* = \frac{\sum_{i=1}^n c_i \vec{v}_i}{\sum_{i=1}^n c_i} \quad (2.1.1-2)$$

where c_i is the concentration of species, i .

In a flowing system, the velocity of a species with respect to all species \vec{v} or \vec{v}^* is of more interest than the velocity with respect to stationary coordinates.

Thus, the useful quantities in such a system would be

$$\vec{v}_i - \vec{v} = \text{Diffusive velocity of } i \text{ with respect to } \vec{v} \quad (2.1.1-3)$$

and

$$\vec{v}_i - \vec{v}^* = \text{Diffusion velocity of } i \text{ with respect to } \vec{v}^* \quad (2.1.1-4)$$

This equation do not worry about the equation numbers. So, these 2 basic definitions we gave and expressed various quantities in terms of the mass average velocity, molar average velocity and so on and so forth.

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The velocity of a species with respect to \vec{v} or \vec{v}^* is of more interest than the velocity with respect to stationary co-ordinates



$$\text{Diffusive velocity of } i \text{ with respect to } \vec{v} = (\vec{v}_i - \vec{v}) \quad \text{Eq. 2.1.1. - 3}$$

$$\text{Diffusion velocity of } i \text{ with respect to } \vec{v}^* = (\vec{v}_i - \vec{v}^*) \quad \text{Eq. 2.1.1. - 4}$$



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Let us consider the disinfection of a laboratory using formaldehyde vapours. Typically, formalin solutions (~40% w/v of formaldehyde in water) is used to generate formaldehyde vapours that kill micro-organisms in an enclosed space. Care is taken to seal all windows and doors with duct tape to prevent leakage of formaldehyde vapours when the disinfection is carried out. The vapours are generated by the increase in temperature due to the exothermic reaction between the added potassium permanganate (KMnO_4) and formalin.



Let us assume that we are generating formaldehyde vapours in a long cylinder. A = formaldehyde (MW=30) and B = air (MW=29). Let us consider the plane where $x_A = 1/5$. Let us say that at that plane,

$$\vec{v}^* = 7 \text{ units} \quad \vec{v}_A - \vec{v}^* = 8 \text{ units}$$


$$\text{Find } \vec{v}_{A,s}, \vec{v}_{B,s}, \vec{v}_B - \vec{v}_s, \vec{v}_{s,b}, \vec{v}_A - \vec{v}_s, \vec{v}_B - \vec{v}$$



We went through a few exercises of those.

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Solution



$$\vec{v}^* = \frac{\sum_{i=1}^n c_i \vec{v}_i}{\sum_{i=1}^n c_i} = \frac{1}{(c_A + c_B)} (c_A \vec{v}_A + c_B \vec{v}_B) = x_A \vec{v}_A + x_B \vec{v}_B$$

x is the mole fraction

From the problem statement we know that at the plane $x_A = \frac{1}{5}$,

$\vec{v}^* = 7$ units (upward direction is taken as positive)

$\vec{v}_A - \vec{v}^* = 8$ units

From the above velocities, we can get


$\vec{v}_A = 8 + \vec{v}^* = 15$ units

Using $\vec{v}^* = x_A \vec{v}_A + x_B \vec{v}_B$ we can get **pause**

$$7 = \frac{1}{5} (15) + (1 - \frac{1}{5}) \vec{v}_B$$

$\therefore \vec{v}_B = 5$ units

$\therefore \vec{v}_B - \vec{v}^* = -2$ units (opposite direction)




Okay we applied it to a situation that normally happens in the lab and that has been our approach you know integrate the problem solving, looking at things from the point of view of problems and so on and so forth. As a part of the basic learning itself.

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We know that $M_A = 30$ (HCHO) and $M_B = 29$ (air)


Let us recognize



$$\vec{v} = \frac{\sum_{i=1}^n \rho_i \vec{v}_i}{\sum_{i=1}^n \rho_i} = \frac{1}{(\rho_A + \rho_B)} (\rho_A \vec{v}_A + \rho_B \vec{v}_B) \quad \text{Eq. 2.1.1.-5}$$

Also, the mass fraction of A is defined as $W_A = \frac{m_A}{(m_A + m_B)}$ Eq. 2.1.1.-6

If we divide the RHS by V , both in the numerator and in the denominator, we get



Then, we said there are 2 basic approaches to solve the relevant problems, okay, typically, we look for concentration profiles, when we solve mass balance, when we apply mass balance to these situations, because concentration profiles give us a lot of useful information. So, to do that, there are 2 major approaches.

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Mass Flux – Shell Balances Approach



One is the shell balances approach.

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Generally speaking, there are two approaches to solve the relevant problems

- (i) the shell balance approach and*
- (ii) the application of the relevant conservation equation*

e.g. the equation of continuity in this case of mass conservation




And the other one is the application of the relevant conservation equation approach. We said that the shell balance approach gives us good physical field for the situation. However, in geometries that are different from the rectangular Cartesian coordinate systems, they could get cumbersome and therefore, we looked at a relevant conservation equation that was reasonably gentle, which could be derived which could be set aside in a table.

And that can be referred to directly, you take that equation cancel out the terms it becomes a risk to be kind of a thing that you could do, much easier to work with. So, that is the relevant conservation equation approach. In the case of cell balances, we did balances over a representative shell in the fluid.

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Shell balances





Balances of conserved quantities are made over a representative shell in the system

The shell represents the geometry under consideration.


For rectangular Cartesian coordinate systems: the shell could be a cuboid
 For cylindrical systems: the shell could be an annular cylinder
 For spherical coordinates: the shell could be an annular sphere.

Let us consider a uniform membrane
 In that membrane, let us consider a shell of thickness Δx , through which diffusion occurs normal to the surface area A

Balances over of conserved quantities are made over a representative shell in the system. The shell depends on the geometry under concentration and so on and so forth. So, here we had looked at a uniform membrane, diffusion through a uniform membrane, and the shell was a part of the membrane therefore, it was a thin cuboid in a membrane itself with a differential cuboid in a membrane of thickness Δx .

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Mass conservation: $\frac{d(m)}{dt} = r_i - r_o + (r_g - r_c)$


A material balance written over the shell (system) on component i entering at x and leaving at $x + \Delta x$ in terms of molar fluxes:

$$\frac{\partial c_i(MW_i)}{\partial t} A \Delta x = N_i|_x(MW_i)A - N_i|_{x+\Delta x}(MW_i)A + R_i(MW_i)A \Delta x \quad \text{Eq. 2.3.1.-1}$$

Let us divide throughout by $(MW_i)A$, a constant in this case **pause**

$$\frac{\partial c_i}{\partial t} = \frac{N_i|_x - N_i|_{x+\Delta x}}{\Delta x} + R_i$$

In the limit $\Delta x \rightarrow 0$, from the definition of the derivative **pause**

$$\frac{\partial c_i}{\partial t} = - \frac{\partial N_i}{\partial x} + R_i \quad \text{Eq. 2.3.1.-2}$$


Over which we wrote our mass conservation balance. Then we wrote the balance in terms of the quantities that we have a handle on in terms of fluxes, molecular mass and so on. Even fluxes become a little difficult. Therefore, we wanted fluxes in terms of concentration and so on.

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Here, the flux N_i is only diffusive

$$\bar{N}_i = \bar{J}_i = -D_i \frac{\partial c_i}{\partial x}$$

Thus

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} + R_i \quad \text{Eq. 2.3.1-3}$$

If there is no net production of i in the volume, Δx , by a reaction



$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} \quad \text{Eq. 2.3.1-4}$$

Fick's second law

Under steady-state conditions **pause**

$$0 = D_i \frac{\partial^2 c_i}{\partial x^2} \quad \text{Eq. 2.3.1-5}$$

In 3-D

$$\frac{\partial c_i}{\partial t} = 0 = D_i \nabla^2 c_i \quad \text{Eq. 2.3.1-6}$$



So, we derived the mass balance equation in detail. And for this situation, we could look at the concentration profile as well as the Fick's second law,

Under steady state conditions (no time dependence i.e. concentration does not vary with time), the LHS of Eq. 2.3.1-4 becomes zero. Thus

$$0 = D_i \frac{\partial^2 c_i}{\partial x^2} \quad (2.3.1-5)$$

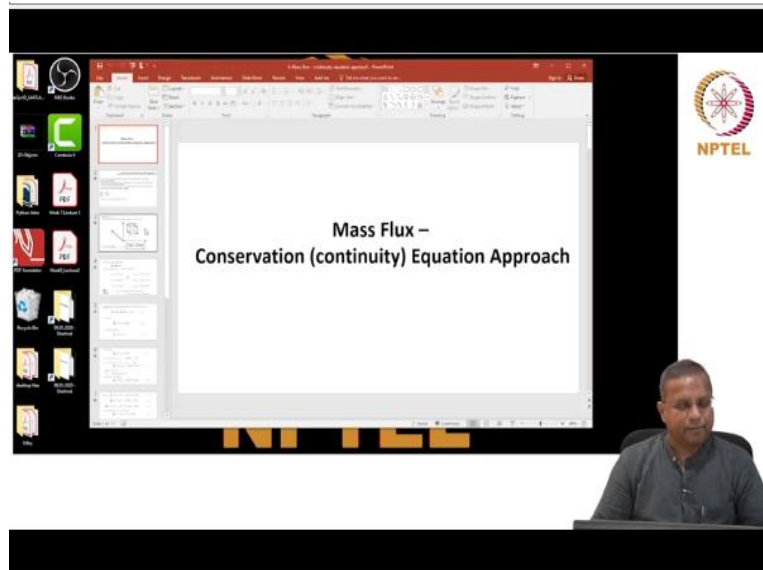
Equation 2.3.1-5 is the one-dimensional diffusion equation under steady state conditions with no reaction.

In three dimensions, under the same conditions, Fick's second law can be written as

$$\frac{\partial c_i}{\partial t} = 0 = D_i \nabla^2 c_i \quad (2.3.1-6)$$

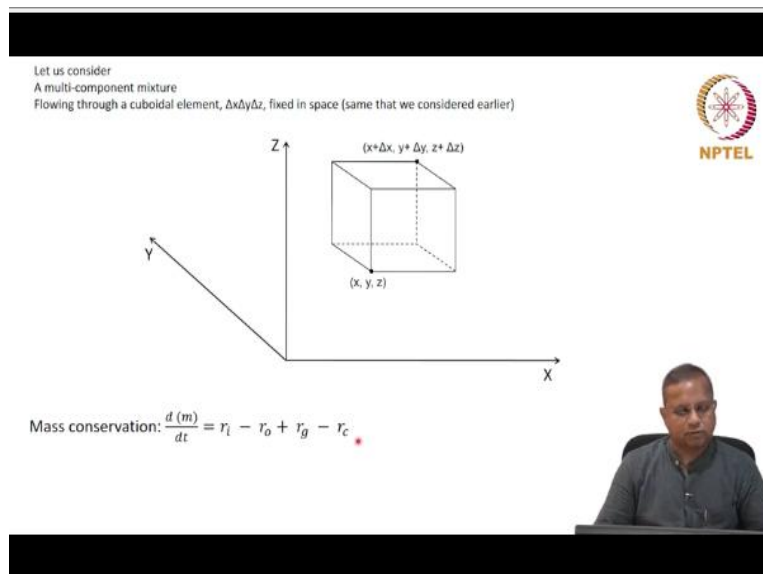
This is the governing equation which is called Fick's second down. Then, under steady state conditions, we saw the concentration profile of the species in the membrane in the system of interest.

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Then after deriving this equation, this is shell balances then we derive the equation let me show just the outlines of the derivation.

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We are considered the rectangular Cartesian coordinate system. And same system as earlier in this case, we are considered a species. When we consider the species there could be an input, there could be an output, there could be generation of the species due to reaction, or there could be a consumption of the species due to reaction.

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For a species, i , in the multi-component mixture,

$$\frac{\partial A_i}{\partial t} = \frac{\partial \rho_i}{\partial t} \Delta x \Delta y \Delta z$$

Note that flux, n_i is a vector. Thus, $\vec{n}_i = \vec{i}n_{ix} + \vec{j}n_{iy} + \vec{k}n_{iz}$



$r_{i,i}|_x = (n_{ix})|_x \Delta y \Delta z$ $r_{i,o}|_{x+\Delta x} = (n_{ix})|_{x+\Delta x} \Delta y \Delta z$

pause

$r_{i,i}|_y = (n_{iy})|_y \Delta x \Delta z$ $r_{i,o}|_{y+\Delta y} = (n_{iy})|_{y+\Delta y} \Delta x \Delta z$

$r_{i,i}|_z = (n_{iz})|_z \Delta x \Delta y$ $r_{i,o}|_{z+\Delta z} = (n_{iz})|_{z+\Delta z} \Delta x \Delta y$

Pause...
What is left over? $r_g - r_c = \text{say, net production rate: } \{R_i (MW_i)\} \Delta x \Delta y \Delta z$
Note: R_i is the rate on a volumetric basis.

And then we derived a general enough relationship by considering all those.
(Refer Slide Time: 21:28)



Substituting in the mass conservation equation, dividing throughout by the volume element $\Delta x \Delta y \Delta z$, and taking the limit as $\Delta x \rightarrow 0, \Delta y \rightarrow 0, \Delta z \rightarrow 0$, we get

$$\frac{\partial \rho_i}{\partial t} + \left(\frac{\partial n_{ix}}{\partial x} + \frac{\partial n_{iy}}{\partial y} + \frac{\partial n_{iz}}{\partial z} \right) = R_i (MW_i) \quad \text{Eq. 2.3.2-1}$$

In vector notation:

$$\frac{\partial \rho_i}{\partial t} + (\vec{\nabla} \cdot \vec{n}_i) = R_i (MW_i) \quad \text{Eq. 2.3.2-2}$$

If we divide throughout by MW,

$$\frac{\partial c_i}{\partial t} + (\vec{\nabla} \cdot \vec{N}_i) = R_i \quad \text{Eq. 2.3.2-3}$$



Okay. In detail, whenever there is a need, you can go through the details to find out.
(Refer Slide Time: 21:32)

Now, let us begin with

$$\frac{\partial \rho_i}{\partial t} + (\vec{v} \cdot \vec{n}_i) = R_i(MW_i) \quad \text{Eq. 2.3.2. - 2}$$

We have already seen (Eq. 2.2.1 - 6) that $-\rho D_i \vec{\nabla} w_i = \vec{n}_i - w_i (\vec{n}_T)$



Substituting \vec{n}_i from Eq. 2.2.1 - 6 in Eq. 2.3.2. - 2, we get **pause**

$$\frac{\partial \rho_i}{\partial t} + (\vec{v} \cdot [w_i (\vec{n}_T) - \rho D_i \vec{\nabla} w_i]) = R_i(MW_i) \quad \text{Eq. 2.3.2. - 4}$$

By definition, $\vec{n}_T = \rho \vec{v}$

Thus, $w_i (\vec{n}_T) = w_i (\rho \vec{v}) = \rho_i \vec{v}$

Therefore, Eq. 2.3.2. - 4 can be written as

$$\frac{\partial \rho_i}{\partial t} + (\vec{v} \cdot [\rho_i \vec{v} - \rho D_i \vec{\nabla} w_i]) = R_i(MW_i) \quad \text{Eq. 2.3.2. - 5}$$



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Reordering, $\frac{\partial \rho_i}{\partial t} + (\vec{v} \cdot (\rho_i \vec{v})) - \vec{v} \cdot (\rho D_i \vec{\nabla} w_i) = R_i(MW_i) \quad \text{Eq. 2.3.2. - 6}$

$$\frac{\partial \rho_i}{\partial t} + (\vec{v} \cdot (\rho_i \vec{v})) - \vec{v} \cdot (D_i \vec{\nabla} \rho_i) = R_i(MW_i) \quad \text{Eq. 2.3.2. - 7}$$

$$\frac{\partial \rho_i}{\partial t} + \rho_i (\vec{v} \cdot \vec{v}) + (\vec{v} \cdot \vec{\nabla} \rho_i) - \vec{v} \cdot (D_i \vec{\nabla} \rho_i) = R_i(MW_i) \quad \text{Eq. 2.3.2. - 8}$$



If ρ and D_i are constants, $(\vec{v} \cdot \vec{v}) = 0$ (Eq. of continuity)

$$\frac{\partial \rho_i}{\partial t} + (\vec{v} \cdot \vec{\nabla} \rho_i) - D_i \nabla^2 \rho_i = R_i(MW_i) \quad \text{Eq. 2.3.2. - 9}$$

Dividing throughout by MW_i

$$\frac{\partial c_i}{\partial t} + (\vec{v} \cdot \vec{\nabla} c_i) - D_i \nabla^2 c_i = R_i \quad \text{Eq. 2.3.2. - 10}$$

Note: \vec{v} is the fluid velocity. **This equation can be used to get concentration profiles - very**

So, this form we said would be useful to us therefore, we express these in individual dimensions. And those became a part of a table in the 3 coordinate systems.

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Table 2.3.2. – 1
The equation of continuity for a species, say i, in a multi-component mixture



Rectangular coordinates:

$$\frac{\partial c_i}{\partial t} + \left(\frac{\partial N_{ix}}{\partial x} + \frac{\partial N_{iy}}{\partial y} + \frac{\partial N_{iz}}{\partial z} \right) = R_i \quad (A1)$$

When c and D_i are constant,

$$\frac{\partial c_i}{\partial t} + \left(v_x \frac{\partial c_i}{\partial x} + v_y \frac{\partial c_i}{\partial y} + v_z \frac{\partial c_i}{\partial z} \right) - D_i \left(\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2} \right) = R_i \quad (A2)$$



So, these were the tables that I showed you and asked you to make a copy of and keep at readily accessible place whenever you are looking at this material. And then I showed you the application of these equations to various situations. The first one was the problem that we solved by shell balances.

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Cylindrical coordinates:

$$\frac{\partial c_i}{\partial t} + \left(\frac{1}{r} \frac{\partial}{\partial r} (r N_{ir}) + \frac{1}{r} \frac{\partial N_{i\theta}}{\partial \theta} + \frac{\partial N_{iz}}{\partial z} \right) = R_i \quad (B1)$$

When c and D_i are constant,

$$\frac{\partial c_i}{\partial t} + \left(v_r \frac{\partial c_i}{\partial r} + v_\theta \frac{1}{r} \frac{\partial c_i}{\partial \theta} + v_z \frac{\partial c_i}{\partial z} \right) - D_i \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c_i}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 c_i}{\partial \theta^2} + \frac{\partial^2 c_i}{\partial z^2} \right) = R_i \quad (B2)$$



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Spherical coordinates:

$$\frac{\partial c_i}{\partial t} + \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 N_{ir}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (N_{i\theta} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial N_{i\phi}}{\partial \phi} \right) = R_i \quad (C1)$$

When c and D_i are constant,

$$\frac{\partial c_i}{\partial t} + \left(v_r \frac{\partial c_i}{\partial r} + v_\theta \frac{1}{r} \frac{\partial c_i}{\partial \theta} + v_\phi \frac{1}{r \sin \theta} \frac{\partial c_i}{\partial \phi} \right) - D_i \left(\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_i}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial c_i}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 c_i}{\partial \phi^2} \right) = R_i \quad (C2)$$



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Now, let us solve the same problem that we did using shell balances earlier, through conservation (continuity) equation. It is best to consider the rectangular Cartesian coordinate system for this situation. Let us choose that equation and cancel the terms that are not applicable. Eq. B from Table 2.3.2 - 1 since c and D_i are constant.



$$\frac{\partial c_i}{\partial t} + \left(v_x \frac{\partial c_i}{\partial x} + v_y \frac{\partial c_i}{\partial y} + v_z \frac{\partial c_i}{\partial z} \right) - D_i \left(\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2} \right) = R_i$$

$\begin{matrix} =0 \text{ (SS)} & =0 \text{ (} v_x = 0 \text{)} & =0 \text{ (} v_y = 0 \text{)} & =0 \text{ (} v_z = 0 \text{)} & =0 \text{ (} c_i \neq f(x) \text{)} & =0 \text{ (} c_i \neq f(y) \text{)} & =0 \text{ (no rxn)} \end{matrix}$

Therefore, $D_i \frac{\partial^2 c_i}{\partial x^2} = 0$

which is the same equation 2.3.1 - 5 we obtained earlier through shell balances

Shell balances, although generally applicable, can sometimes become cumbersome, and thus this conservation equation approach would be convenient to use in many situations

Note that we derived these conservation equations based on standard shells - cuboidal, cylindrical or spherical. If the shell shape is different, for example, if the c.s. area is variable, equations A2, B2, and C2 are not applicable. However, verify that A1, B1, and C1 are not affected by this aspect, and are generally applicable



I showed you how very simply speaking, you just take the equation, you cancel the irrelevant terms. And at one swell step, you get the equation that we got through a lengthy derivation through shell balances, okay, this is the advantage of using one such thing therefore it is already gone into deriving a general enough equation which can be applied. Because this equation does not hold when there is a change in your cross section, over your system of interest and so on and so forth. You need to keep that in mind.

Then, we had applied to various situations. The first one was of course, the rectangle Cartesian coordinate system case, then we had used it to look at steady state diffusion of certain species across walls across membranes, then across tubular walls, we looked at the trachea sorry the bronchiole and a drug distributing from the inside of the bronchiole to the outside.

How do you look at that, and then we looked at diffusion through spherical porous pellets. And then these 3 were without reaction, then we brought in a reaction and looked at an enzymatic reaction where the enzyme is immobilized inside a porous pellet. So, that is the application of the equations to the 3 different geometries. And then we looked at an unsteady case where once you bring in an unsteady term, the time derivative, it complicated the mathematical effort significantly, okay.

And as all those things we saw, the unsteady state case was, we had a protein solution that is solving onto a surface. And we were interested in the concentration profiles in that quiescent liquid about the surface, the variation of the concentration profiles with time. Okay, those are the things that we saw.

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Pseudo-steady state approximation (PSSA)



And finally, let me have been at this for a while, I think we should stop to avoid fatigue. I will just say this. It is important. Then we will stop for today and continue in the next class. Okay. So, we also looked at a very powerful approximation, a very powerful idea, called the pseudo steady state approximation.

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Pseudo-steady state approximation (PSSA) is a view/technique that can be used to simplify the analysis, and the mathematical complexity **when comparing two processes of widely varying rates**

To understand the pseudo steady state approximation, let us consider the process of car manufacture. Let us focus on three of the processes as shown below.



Process	Making the bolts that are used in the engine	Making the engine	Making the whole car
Characteristic rates	Say, 1 bolt per 5 seconds	Say, 1 engine per 1 hour	Say, 1 car per 24 hours

If we focus on engine making, whether the rate of bolt making is 5 s^{-1} or 8 s^{-1} or 2 s^{-1} , ... does not affect the rate of engine making.

If our interest is engine-making, the process of bolt-making is fast enough to be considered at pseudo-steady state, i.e. the changes in the rate of bolt-making (unsteady aspects) will not much affect the rate of engine-making.

Also the rate of whole-car-making is so slow, that it is not even relevant to the rate of engine-making.

Thus, for the interest at hand, i.e. engine-making, the process of whole-car-making can be taken as 'frozen'.

It is something like this when you have, when you are comparing to processes of widely varying rates, the much faster process can be taken to be at steady state, if the interest is this slower process.

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Now, let us consider some cellular processes:

Process	Enzyme action	Cell growth/division	Natural mutation
Characteristic rates	One in every 10^{-3} s	One in every 10^2 s	One in every 10^6 s

If we are interested in cell growth/division, the enzyme action can be taken to be at pseudo steady state, and natural mutation can be considered 'frozen'.



Now, let us consider a thin membrane through which diffusion of a species occurs

Let us take the membrane as the system



Let us say the interest is in the changes in the species concentration in the solutions that are separated by the membrane

If the diffusion through the membrane is fast enough compared to the changes in the concentration of the species in the solutions separated by the membrane, then the diffusion through the membrane can be assumed to take place under steady-state conditions.

So, we had applied this to come up with the permeability of a coating layer, when the permeability through the coating layer is of interest, the experiment that is done as measuring permeability of a mechanically stable membrane, and then you put the coating layer onto the membrane and measure the combined permeability.

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Let us consider the permeability of a model protein (albumin) a coating used to improve cell adherence on surfaces. The permeability can be measured using a cylindrical vessel separated into two chambers, A and B, by the material whose permeability is being measured.



Since the coating is too thin to have the necessary mechanical properties to act as the above mentioned separator between the two chambers, another technique is used to find the needed permeability.

The permeability of a membrane with suitable mechanical properties is first measured. Then, the permeability of the membrane with the 'coating' of interest is measured. The membrane used in the experiment is circular with an area of 1.33 cm^2 and the volume of each chamber (A or B) is 2 cm^3 .

The initial concentration of growth factor in chamber A at the start of the experiment was 10 mg l^{-1} , and no growth factor was initially present in chamber B. The growth factor concentration at different times (in min) in chamber B from the start of experiment are given in mg l^{-1}

Time	Concentration with membrane	Concentration with coated membrane
0	0.0	0.000
20	0.4	0.010
40	0.7	0.020
80	1.3	0.035



Determine the growth factor permeability of the coating. Assume that the flux through the membrane occurs much faster compared to the change in concentrations on both sides of the membrane.

And from that data to extract out the relevant membrane permeability, we had to use the pseudo steady state principle and get the permeability.

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Solution strategy
 Consider the membrane and the coating to be 'membranes in series'
 Thus, their resistances, or inverse of their conductances (permeabilities) are additive
 Permeability is equal to DK/L , where D is the diffusivity, K, the partition coefficient, and L the membrane thickness

That is what we had seen. That was the example that was given. The pseudo steady state concept itself was a very powerful concept that can be use in any situation whenever you compare to processes of widely varying rates and the interest is in the slower process. Okay. I think that is what we did for mass flux, mass transport, mainly through diffusion okay, there is no mass flux through bulk movement.

Although the equations that were derived had the ability to handle that also. But for better understanding, we just forced the driving force to a concentration gradient. In all these cases, we took examples here only the concentration gradient was the driving force, and showed you

the various applications of it. When we come back in the next class, we have been at this for a while now and we come back, we would look at momentum flux, review that and forward. See you in the next class. Bye