Transport Phenomena in Biological Systems

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Lecture-08
Mass and Molar Fluxes

Welcome. Let us continue with our formulation here of mass flux. So, mass flux and molar flux. Earlier we looked at velocities. And now we are going to look at the fluxes.

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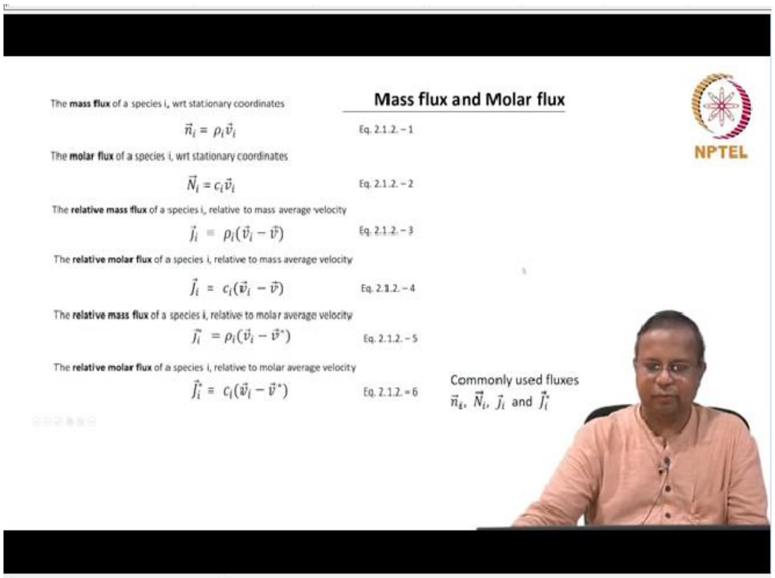


Mass flux and Molar flux

The **mass flux** of a species i, wrt stationary coordinates

$\vec{n}_i = \rho_i \vec{v}_i$ Eq. 2.1.2. – 1

The **molar flux** of a species i, wrt stationary coordinates

$\vec{N}_i = c_i \vec{v}_i$ Eq. 2.1.2. – 2

The **relative mass flux** of a species i, relative to mass average velocity

$\vec{j}_i = \rho_i(\vec{v}_i - \vec{v})$ Eq. 2.1.2. – 3

The **relative molar flux** of a species i, relative to mass average velocity

$\vec{J}_i = c_i(\vec{v}_i - \vec{v})$ Eq. 2.1.2. – 4

The **relative mass flux** of a species i, relative to molar average velocity

$\vec{j}_i^* = \rho_i(\vec{v}_i - \vec{v}^*)$ Eq. 2.1.2. – 5

The **relative molar flux** of a species i, relative to molar average velocity

$\vec{J}_i^* = c_i(\vec{v}_i - \vec{v}^*)$ Eq. 2.1.2. – 6

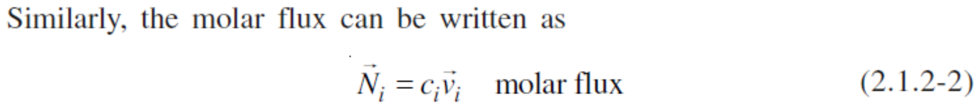
Commonly used fluxes
$\vec{n}_i$, $\vec{N}_i$, $\vec{j}_i$ and $\vec{J}_i^*$

The mass flux of species i with respect to stationary coordinates is nothing but the product of the density (ρ_i) times the velocity(v_i). The symbol that we are going to use is n_i, it is a vector, because it has direction, both magnitude and direction. Therefore, the mass flux of species i represented as n_i is density times velocity, we also already seen the density times velocity is the mass flux.

We will call this equation, 2.1.2 - 1, the mass flux of species i with again with respect to stationary coordinates.

$$\vec{n_i} = \rho_i \vec{v_i} \qquad (2.1.2\text{-}1)$$

We are going to represent molar flux as N_i. So, N_i is nothing but concentration(c_i) times the velocity(v_i). This is the velocity of the species i, we said that we are more interested in the relative movement. This is denoted by equation 2.1.2-2

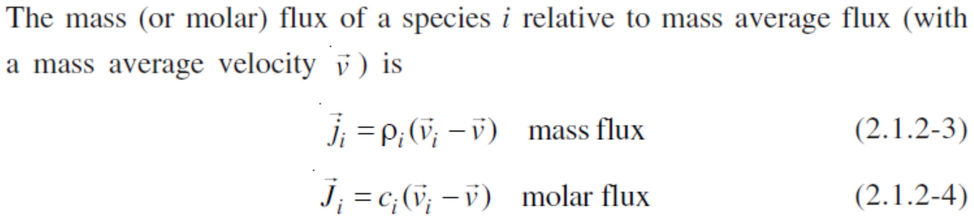


Similarly, the molar flux can be written as

$$\vec{N}_i = c_i\vec{v}_i \quad \text{molar flux} \qquad (2.1.2\text{-}2)$$

Therefore, the relative mass flux of species i (j_i), relative to mass average velocity(v) is denoted as j_i. We are taking the mass average velocity to compare it with that we represent as j_i is ρ_i times the difference of diffusive velocity v_i and the mass average velocity v and we have taken the difference here v_i - v presented in the equation 2.1.2 – 3,($j_i = \rho_i (v_i - v)$).

The relative molar flux of species i relative to the mass average velocity(v) is represented as capital J_i. And that is nothing but concentration(c_i) times the velocity difference $v_i - v$. Again, the average with respect to mass average velocity or the relationship with respect to mass average velocity is given in 2.1.2 – 4, ($J_i = c_i (v_i - v)$). Only couple more these are the standard ones, so I am listing them all together.



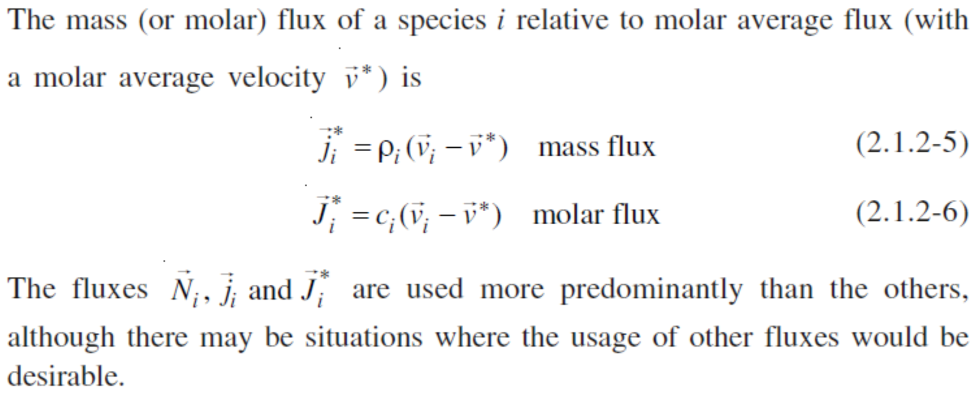
The mass (or molar) flux of a species *i* relative to mass average flux (with a mass average velocity $\vec{v}$) is

$$\vec{j}_i = \rho_i(\vec{v}_i - \vec{v}) \quad \text{mass flux} \qquad (2.1.2\text{-}3)$$

$$\vec{J}_i = c_i(\vec{v}_i - \vec{v}) \quad \text{molar flux} \qquad (2.1.2\text{-}4)$$

And these are rather simple, flux is nothing but density times velocity, molar versus concentration times velocity, here it is only a diffusive aspect or the relative mass flux that we are looking at. Now the relative mass flux of species i (j_i^*) relative to molar average velocity (v^*) is going to be j_i^* that is $j_i^* = \rho_i (v_i - v^*)$ (2.1.2 – 5).

The relative molar flux of species i (J^*_i), relative to the molar average velocity (v^*) is c_i times the diffusive velocity with respect to the molar average velocity ($v_i - v^*$) (2.1.2 – 6). We are going to use these frequently some of these frequently, I think I have listed. Yeah, the commonly used fluxes are the mass flux n_i, the molar flux N_i, the relative mass flux, j_i and the relative molar flux $J^* = c_i(v_i - v^*)$.



The mass (or molar) flux of a species i relative to molar average flux (with a molar average velocity $\vec{v}^*$) is

$$\vec{j}_i^* = \rho_i(\vec{v}_i - \vec{v}^*) \quad \text{mass flux} \qquad (2.1.2\text{-}5)$$

$$\vec{J}_i^* = c_i(\vec{v}_i - \vec{v}^*) \quad \text{molar flux} \qquad (2.1.2\text{-}6)$$

The fluxes $\vec{N}_i$, $\vec{j}_i$ and $\vec{J}_i^*$ are used more predominantly than the others, although there may be situations where the usage of other fluxes would be desirable.

These are the ones that we will commonly use in this course. There are various other basis on which you can take relative fluxes on a molar basis and so on and so forth. If it is necessary, you can always go and pick it up from other books or you can just extend this formulation to other things, we would not be using those fluxes much and therefore I have not listed them here. There are many other bases on which you can take the relative fluxes, mass fluxes and molar fluxes. We do not get into that in this course.

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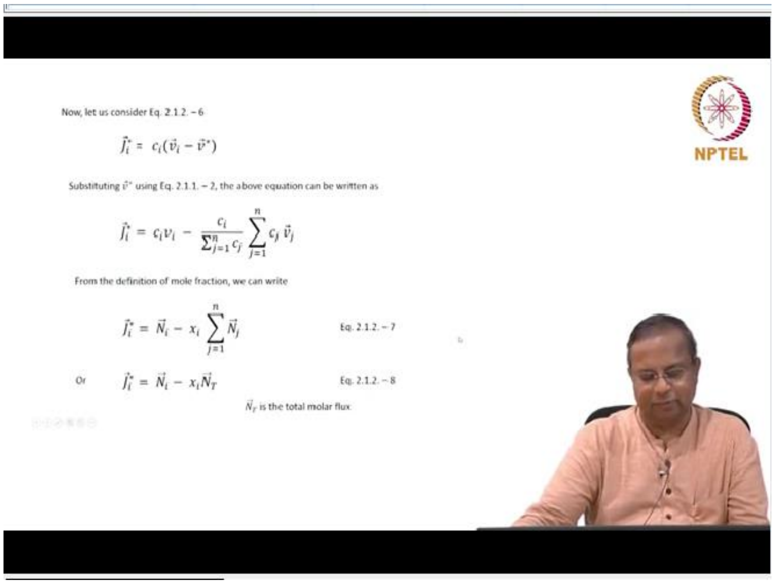


Now, let us consider Eq. 2.1.2. – 6

$$\vec{J}_i^* = c_i(\vec{v}_i - \vec{v}^*)$$

Substituting $\vec{v}^*$ using Eq. 2.1.1. – 2, the above equation can be written as

$$\vec{J}_i^* = c_i v_i - \frac{c_i}{\sum_{j=1}^{n} c_j} \sum_{j=1}^{n} c_j \vec{v}_j$$

From the definition of mole fraction, we can write

$$\vec{J}_i^* = \vec{N}_i - x_i \sum_{j=1}^{n} \vec{N}_j \qquad \text{Eq. 2.1.2. – 7}$$

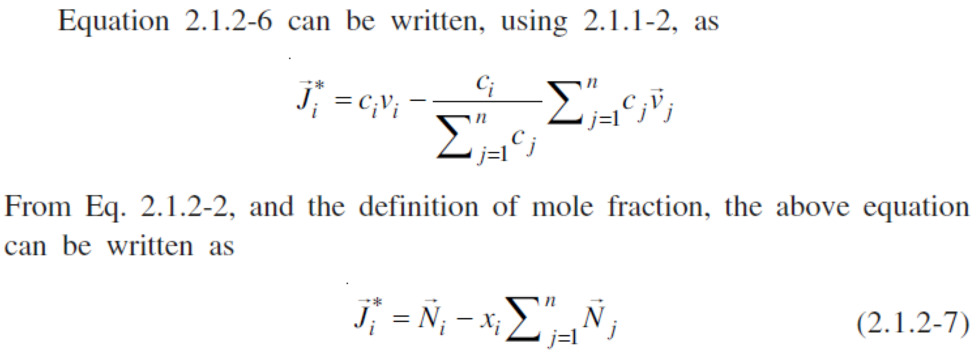
Or

$$\vec{J}_i^* = \vec{N}_i - x_i \vec{N}_T \qquad \text{Eq. 2.1.2. – 8}$$

$\vec{N}_T$ is the total molar flux

$$\bar{v} = \frac{\sum_{j=1}^{n} c_j \overline{v_j}}{\sum_{j=1}^{n} c_j} \qquad 2.1.1\text{-}2$$

Now substitute for v* from equation 2.1.1-2 into the equation 2.1.2 – 6. If you substitute for v* using the definition of v* from 2.1.1-2 which is summation of c_j v_j divided by the summation of c_j. We get $c_i v_i$ – c_i v* in 2.1.2-6. And from the definition of mole fraction, concentration divided by the total concentration can be written as x_i. N_i, molar flux is c_i v_i from equation 2.1.2-2

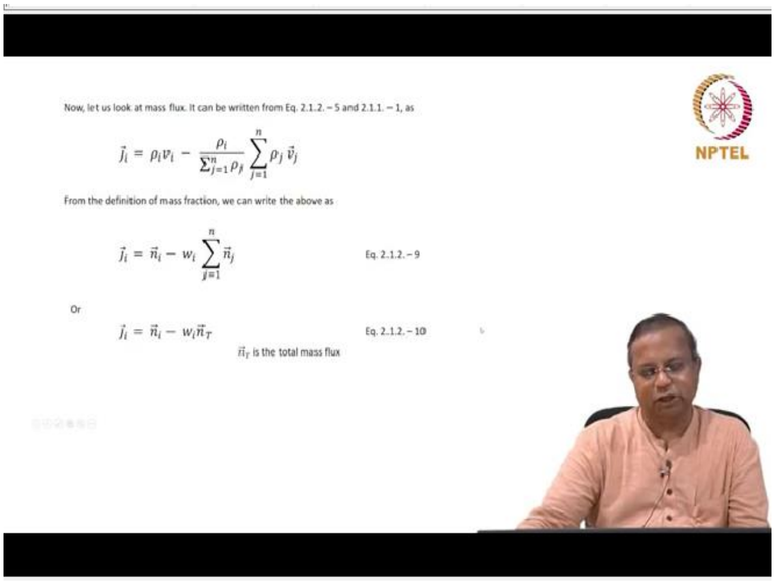


Equation 2.1.2-6 can be written, using 2.1.1-2, as

$$\vec{J}_i^* = c_i v_i - \frac{c_i}{\sum_{j=1}^{n} c_j} \sum_{j=1}^{n} c_j \vec{v}_j$$

From Eq. 2.1.2-2, and the definition of mole fraction, the above equation can be written as

$$\vec{J}_i^* = \vec{N}_i - x_i \sum_{j=1}^{n} \vec{N}_j \qquad (2.1.2\text{-}7)$$



Now, let us look at mass flux. It can be written from Eq. 2.1.2. – 5 and 2.1.1. – 1, as

$$\vec{j}_i = \rho_i v_i - \frac{\rho_i}{\sum_{j=1}^{n} \rho_j} \sum_{j=1}^{n} \rho_j \vec{v}_j$$

From the definition of mass fraction, we can write the above as

$$\vec{j}_i = \vec{n}_i - w_i \sum_{j=1}^{n} \vec{n}_j \qquad \text{Eq. 2.1.2.} - 9$$

Or

$$\vec{j}_i = \vec{n}_i - w_i \vec{n}_T \qquad \text{Eq. 2.1.2.} - 10$$

$\vec{n}_T$ is the total mass flux

This is nothing but the sum of all molar fluxes and that we are going to represent it as N_T is a total molar flux and we will call this equation 2.1.2 - 8.

J_i* = N_i – x_i N_T 2.1.2-8

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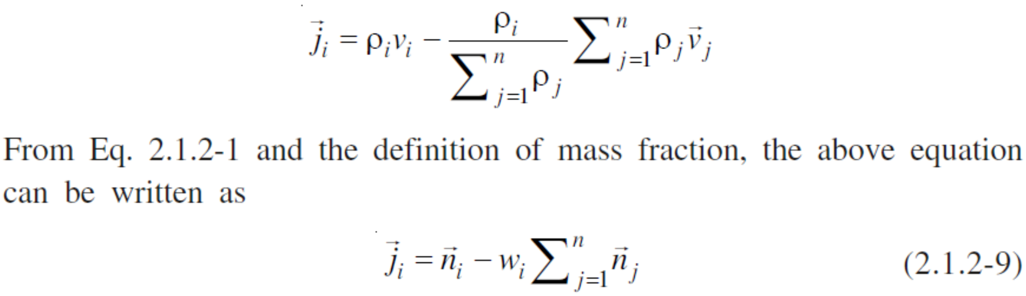
Now let us look at mass flux. The 2.1.2 - 5, which is this lowercase j yeah, this is a lowercase j this mass flux right lower case j_i* because it is with relative to molar average velocity is ρ_i times

v_i - v^*. And if you look at this J is ρ_i v_i - sum of ρ_j v_j divided by the sum of ρ_j. And because we have removed the brackets ρ_i comes up here. You can see where I am getting at, this is nothing but the mass fraction. So, from the definition of mass fraction, mass fraction is mass of i divided by the total mass, you divide above and below by volume, you will get density divided by the total density right. Therefore, j_i is n_i – w_i times the sum over n_j, of all the other mass fluxes, all different mass fluxes. We will call this equation 2.1.2 - 9



$$\vec{j}_i = \rho_i v_i - \frac{\rho_i}{\sum_{j=1}^{n} \rho_j} \sum_{j=1}^{n} \rho_j \vec{v}_j$$

From Eq. 2.1.2-1 and the definition of mass fraction, the above equation can be written as

$$\vec{j}_i = \vec{n}_i - w_i \sum_{j=1}^{n} \vec{n}_j \qquad (2.1.2\text{-}9)$$

j_i is nothing but n_i – w_i n_T, this is n_T, the total mass flux, that is been written here, this is equation 2.1.2 - 10 .

$j_i = n_i - w_i\, n_T$ 2.1.2-10

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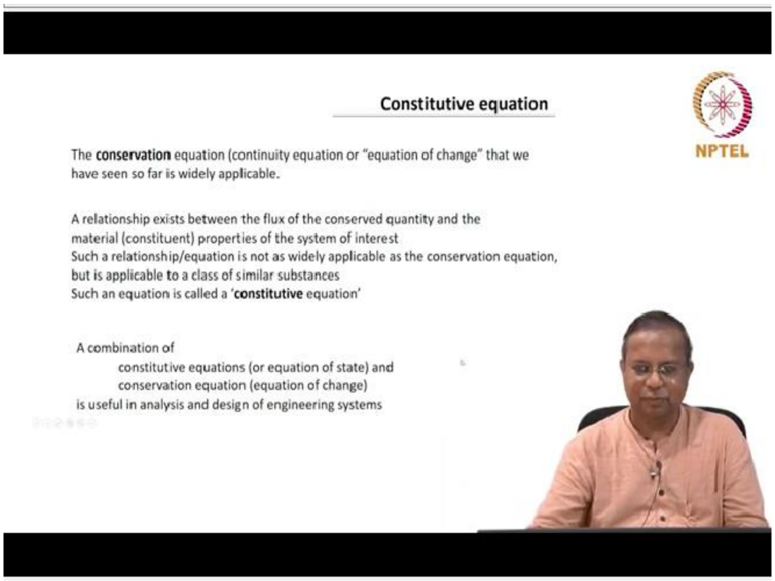

Constitutive equation

The **conservation** equation (continuity equation or "equation of change" that we have seen so far is widely applicable.

A relationship exists between the flux of the conserved quantity and the material (constituent) properties of the system of interest
Such a relationship/equation is not as widely applicable as the conservation equation, but is applicable to a class of similar substances
Such an equation is called a '**constitutive** equation'

A combination of
constitutive equations (or equation of state) and
conservation equation (equation of change)
is useful in analysis and design of engineering systems

So, these are some ways of these expressions will turn out to be useful. That is the reason I wrote these here. Let us continue. I think yeah we have been at for not too long time so we can continue a little further. We will talk about a constitutive equation is a different concept. We have seen conservation equation so far, the mass conservation equation, mass conservation equation in the context of whatever we did became what is called the continuity equation .

That is an equation of change, it tells you how the mass changes over time. And that is widely applicable, the only riders that we put on us, no nuclear conversions or no nuclear reactions and no traveling at the speeds close to that of light. So, very widely applicable for most of our or almost all our applications. A relationship exists between the flux of the conserved quantity here.

And the material or the constituent properties of the system of interest usually. Such a relationship is not as widely applicable as the conservation equation, we cannot close your eyes and apply it, but it is applicable to a wide variety of substances or a class of similar substances, and therefore that turns out to be useful. And that is called a constitutive equation, a conservation equation typically mass conservation, momentum conservation, energy conservation, charge conservation are very widely applicable.

Almost across the board, whereas the constitutive equation is a relationship between the flux of a conserved quantity and the material properties of the system of interest. That is not as widely applicable as a conservation equation, but it is still applicable over a wide range of substances of similar substances. And since it is related to the constituent properties, we call it the constitutive equation. A combination of the constitutive equations are equations of state, a constitutive equation as the equation of state, do you recall equation of state now, think about it.

And conservation equation equations of change, constitutive equations of state $P V = n R T$ is an equation of state and conservation equation, equation of change the mass conservation equation is useful in analysis and design of engineering systems. So this pretty much is another base for this course, we are going to see this in various different aspects of this course. The combination of constitutive equations and conservation equations for each different case.

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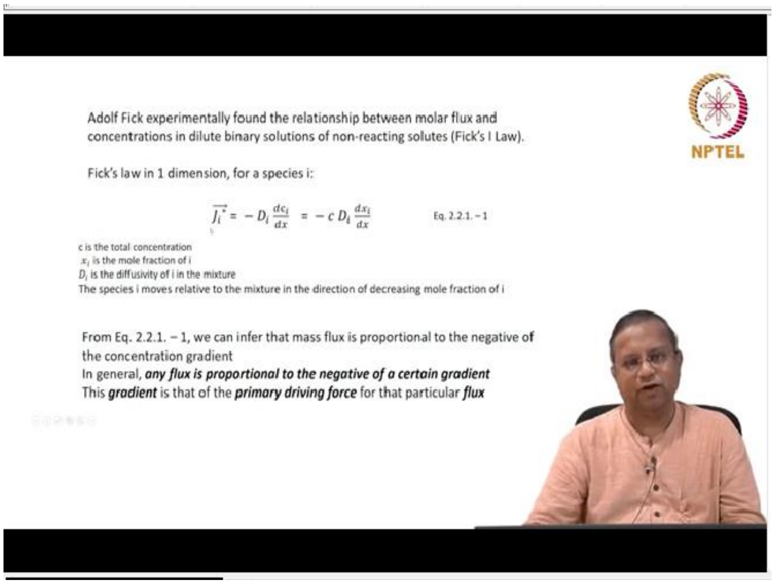

Adolf Fick experimentally found the relationship between molar flux and concentrations in dilute binary solutions of non-reacting solutes (Fick's I Law).

Fick's law in 1 dimension, for a species i:

$$\overrightarrow{J_i^*} = -D_i \frac{dc_i}{dx} = -c\, D_i \frac{dx_i}{dx} \qquad \text{Eq. 2.2.1.} - 1$$

c is the total concentration
x_i is the mole fraction of i
D_i is the diffusivity of i in the mixture
The species i moves relative to the mixture in the direction of decreasing mole fraction of i

From Eq. 2.2.1. – 1, we can infer that mass flux is proportional to the negative of the concentration gradient
In general, ***any flux is proportional to the negative of a certain gradient***
This ***gradient*** is that of the ***primary driving force*** for that particular ***flux***

Adam Fick experimentally found the relationship between molar flux and concentrations in dilute binary solutions of non reacting solutes, . The conditions are important, relationship between molar flux and concentrations, dilute binary solutions binary solutions to components of non reacting solutes. And he experimentally found this out first and came up with Ficks first law. Ficks first line one dimension for a species i is nothing but the molar flux of i = $D_i \left(-\frac{dc_i}{dx}\right)$.

Let me take the minus along with this where it actually belongs D_i times - $\frac{dc_i}{dx}$. $\frac{dc_i}{dx}$ is nothing but the concentration gradient, the variation of concentration with respect to space. Single dimension x. If this is c_i, you could write it in terms of the mole fraction right, so c times x_i is c_i ($cx_i=c_i$) c is a constant the total concentration is a constant of all the species taken together and if we can bring it out of the derivative, that we can write this as

$$\mathbf{J_i^* = D_i \left(-\frac{dc_i}{dx}\right) = -\,c\, D_i \frac{dx_i}{dx}} \qquad \mathbf{2.2.1\text{-}1}$$

Note that this is mole fraction, this is the x dimension . There is a possibility of a confusion here, do not worry about it, $\frac{dx_i}{dx}$ the variation of with respect to x of the mole fraction. This is an important equation in the constitutive equation, Fick's first law, which relates the molar flux with the concentration in dilute binary relations. We call this equation 2.2.1 - 1. This D_i, the capital D_i is called the diffusivity of i in the mixture .

This although written for binary solution, you can extend it to multicomponent mixtures also, that is the reason I put an D_i here, rather than a D_{AB} or something like that to generalize it to multicomponent mixture. So, D_i is the diffusivity of i, in the mixture. The species, i most related to the mixture in the direction of decreasing mole fraction of i , that is the reason why there is a negative here , the flux is proportional to the negative of the concentration gradient.

Yeah, that is what that is given here mass flux is proportional to the negative or the concentration gradient. In general, any flux is proportional to the negative of a certain gradient, that is what it will turn out to be. And we will look at them one by one, as we go along. This gradient is that of the primary driving force for that flux , in this case, you have the concentration gradient, the concentration gradient is proportional to the flux.

The flux is proportional to the concentration gradient. That is the way to look at it in terms of independent and dependent quantities. And this concentration gradient happens to be the primary driving force for the mass flux.

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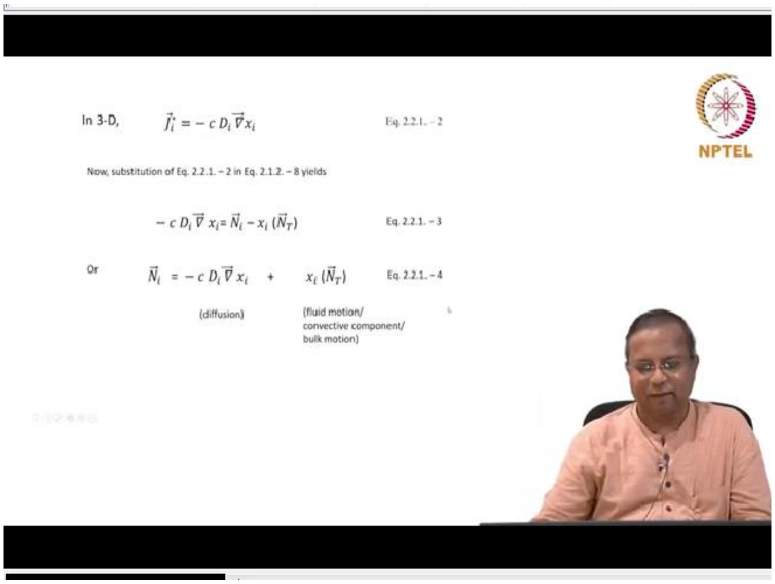

In 3-D, $\vec{J}_i^* = -c\,D_i \vec{\nabla} x_i$ Eq. 2.2.1. - 2

Now, substitution of Eq. 2.2.1. – 2 in Eq. 2.1.2. – 8 yields

$-c\,D_i \vec{\nabla}\, x_i = \vec{N}_i - x_i\,(\vec{N}_T)$ Eq. 2.2.1. – 3

Or $\vec{N}_i = -c\,D_i \vec{\nabla}\, x_i + x_i\,(\vec{N}_T)$ Eq. 2.2.1. – 4

(diffusion) (fluid motion/ convective component/ bulk motion)

In 3-dimensions, this is only one dimension, we are looking at the general formulations in this course in 3-dimensions is as practical as we can get practical and as gentle as we can get for our situations. You could replace the derivative here, $\frac{d}{dx}$ with a ∇ right. So, in the three-dimension, we get, $\mathbf{J_i^* = - c\, D_i\, \nabla x_i}$ **2.2.1 - 2.**

Now if you substitute 2.2.1 - 2 and 2.1.2 - 8, which is this $J_i^* = N_i - x_i N_T$, we get,

$\mathbf{- c\, D_i\, \nabla\, x_i = N_i - x_i\, N_T}$ **2.2.1 - 3**

Rearranging the above equation, keeping N_i on one side, we get,

$\mathbf{N_i = - cD_i\, \nabla\, x_i + x_i\, N_T}$ **2.2.1 – 4**

$cD_i\, \nabla\, x_i$ - this is the molar flux due to diffusion or molecular motion and $x_i\, N_T$ - this is the molar flux resulting from fluid motion convective motion or the bulk motion, recall. Stirring of your tea, coffee, the sugar in your tea or coffee with a spoon. That is a fluid motion- convective motion or bulk motion, these are terms that we are going to use to represent that stirring equally.

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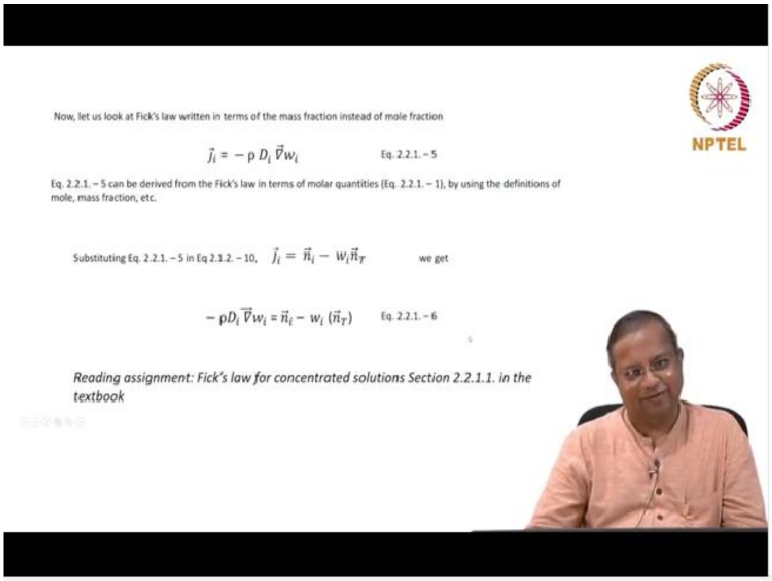

Now, let us look at Fick's law written in terms of the mass fraction instead of mole fraction

$$\vec{j}_i = -\rho\, D_i\, \vec{\nabla} w_i \qquad \text{Eq. 2.2.1.-5}$$

Eq. 2.2.1. – 5 can be derived from the Fick's law in terms of molar quantities (Eq. 2.2.1. – 1), by using the definitions of mole, mass fraction, etc.

Substituting Eq. 2.2.1. – 5 in Eq 2.1.2. – 10, $\vec{j}_i = \vec{n}_i - w_i \vec{n}_T$ we get

$$-\rho D_i\, \vec{\nabla} w_i = \vec{n}_i - w_i\, (\vec{n}_T) \qquad \text{Eq. 2.2.1.-6}$$

Reading assignment: Fick's law for concentrated solutions Section 2.2.1.1. in the textbook

Let us see the Fick's law written in terms of mass fraction, instead of the mole fraction . We can do that either way. So, you can actually derive this, and I am just going to say this

$\mathbf{j_i}$ **(mass flux of i)=** $- \rho D_i \nabla w_i$ **2.2.1 - 5**

Why do not I let you derive this if you run into difficulties with this derivation then get back to me, send me an email. I will tell you how to do it. This is a few steps and it is good for you to go back. It is just definition and do the various definitions and you get from there with our Fick's first law in terms of mole fractions.

Now if you substitute 2.2.1-5 in 2.1.2 - 10, which is $\mathbf{j_i = n_i - w_i\, n_T}$, we get you know j_i we are replacing equation by

$- \rho D_i \nabla w_i = n_i - w_i\, n_T$ **2.2.1 - 6**

And this all these are useful expressions. So, that is the reason why we have derived this and how it turned out to be useful. We will see in the later courses or later classes of this course. I am going to leave this as a reading assignment for you. What is reading assignments do is they will expand your understanding, make them more complete. Most of them will be from the textbook. However, given the access I am not going to make that compulsory in other words you would not be tested on those for people who are worried about being tested and so on and so forth. It is a very common concern. You would not be tested on these reading assignments here.

But it is good for you to understand the material, so go find the book and read this. What I would like you to read from the book is Fick's law for concentrated solutions. Recall that the earlier formulation of the Fick's law all these are for dilute solutions, that is what Fick did. And in our biological case, you would very rarely find dilute solutions, most of them would be concentrated.

And you could come up with a slightly different formulation for this for concentrated solutions in terms of chemical protection. And that is given in section 2.2.1. 1 in the textbook. Go and read that books. I think we will stop here yeah we are at the end we will stop here for this lecture and continue in the next lecture, see you.