Transport Phenomena in Biological Systems
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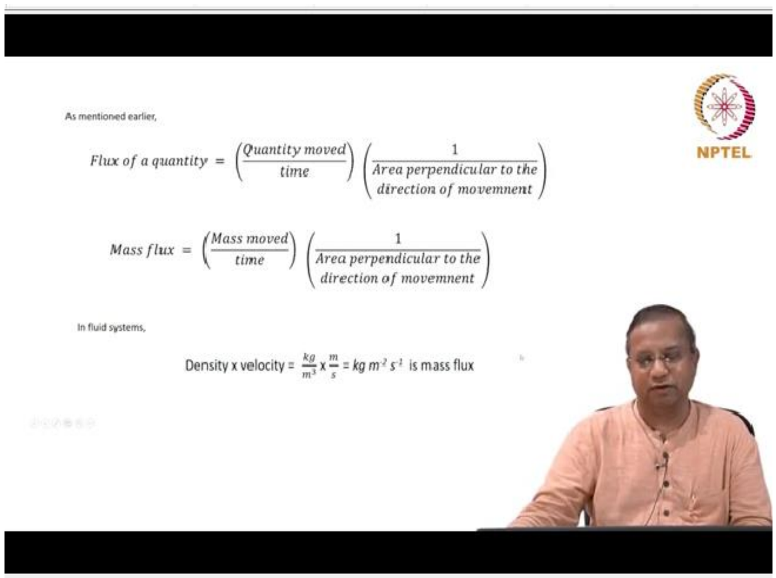
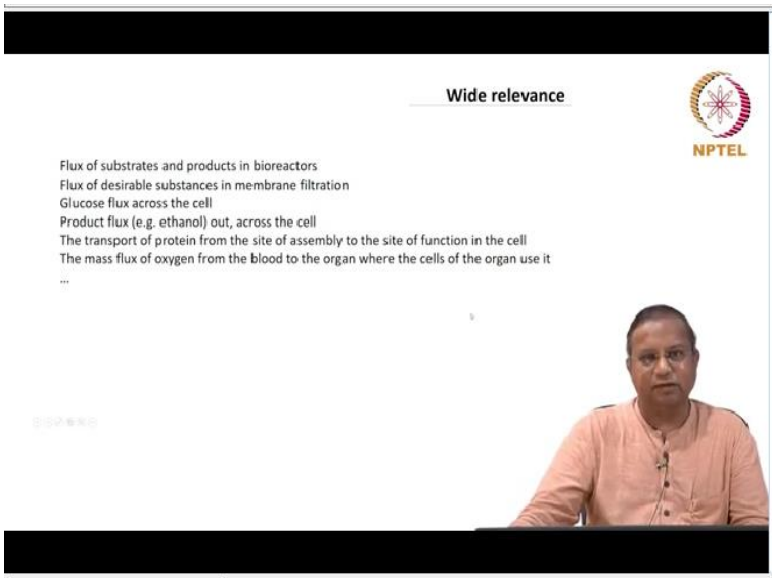
Lecture-07
Mass Flux

Welcome back. Today, let us begin the flux aspects. We begin with mass flux. Earlier, we saw some applications of mass conservation. And today, we are getting into the actual theme or actual concept of this course, which are fluxes and the forces that cause these fluxes. Let us begin with mass flux.



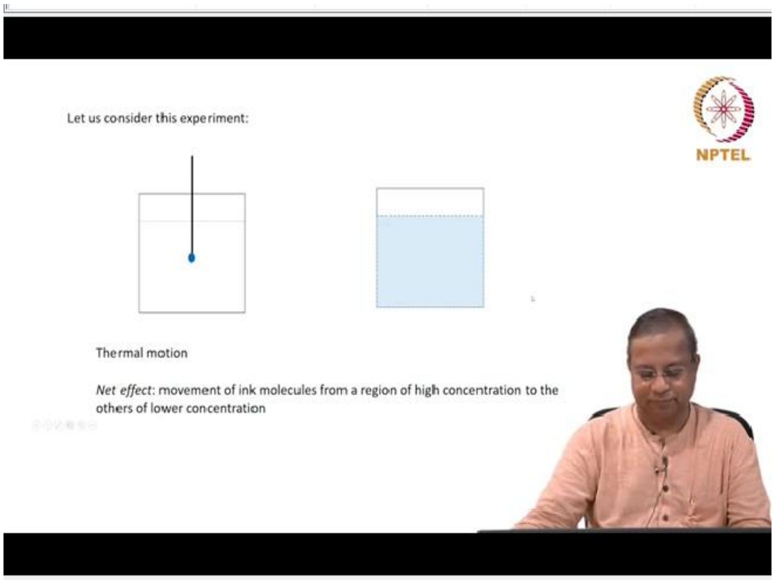
We have already seen that flux of conserved quantity in this case is the quantity moved per time, normalized with respect to the area perpendicular to the direction of movement. For example, mass flux is mass moved per time, divided by the area. All our formulations are in terms of fluxes that makes it easier to formulate across various things and that is the reason why we are sticking to this quantity flux.

And that is the historical development and therefore we are sticking to that quantity. In fluid systems we saw that the product of the density and velocity turned out to be mass flux. You can see the units here, which also give a good indication, the units of density are kilogram per meter cube, that of velocity is meter per second. And therefore, you get kilogram per meter square per second or kilogram per second per meter square for mass flux.



It has wide relevance, of course, the flux of substrates and products in bioreactors is very important. Just giving you some examples here. The application is wide, anything that you can think of, will have movement of substances or any dynamic system will have movement of substances and therefore flux is important. Some examples are flux of substrates and products in bioreactors, flux of desirable substances in membrane filtration in the downstream processing aspects. If you are looking at a bioprocess, glucose flux across the cell, which is essential for the energy of the cell, the product flux, in this case, for example ethanol moving out of the cell into the extracellular space and that is what makes it easier to process ethanol. The transport of protein from the site of assembly to the site of function within the cell itself, microscopic cell. You know, transcription, translation and then there are steps after translation. Then there is transport of protein to the area of interest or the area of its function, the point of its function in the cell. So, the transport of protein from the site of assembly to the site of function in the cell is relevant. The mass flux of oxygen from the blood to the organ where the cells of the organ use it. You can think of various different things.

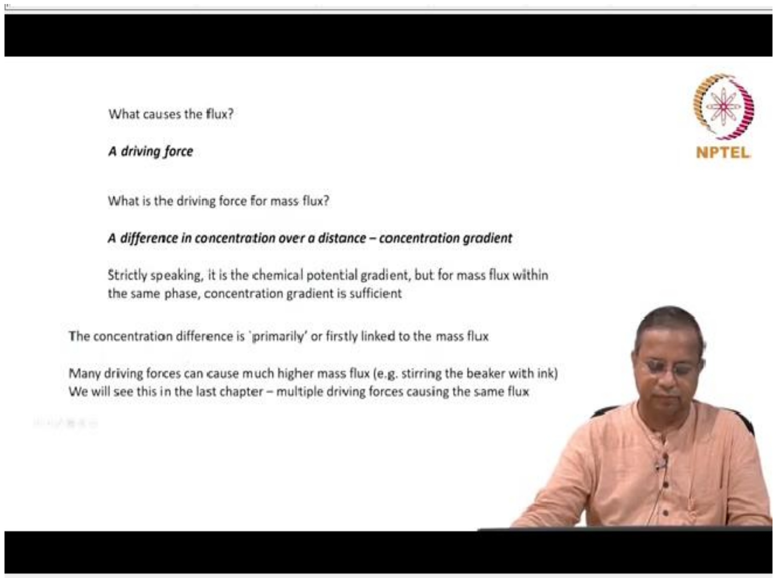
From now onwards you start looking at various aspects in terms of what flux is. That would give you a better appreciation of the applications of this course, the applications are wide, this is limited by the sun, I suppose and in a regular class in a face to face class that we have something called a CFA exercise that brings this point across by getting the students themselves to think about the various applications and make a semester long project out of it. That is not possible in this framework except in a certain minor way, which I think I have mentioned earlier. So, the applications are wide. So, let us start looking at them.



Let us consider this experiment first. We have a vessel, a vessel which has liquid, let us say water. And we carefully take a pipette filled with ink. And when we reach somewhere in the center, we release a drop of ink, which is colored blue indigo in this case into the liquid. If you just drop the liquid and leave it aside. And then wait, come back after some time, a long time and check the drop of ink would have uniformly distributed across the entire liquid, just by sitting still.

And therefore, something has moved the ink droplets or ink molecules from the point of its release to the entire liquid. If the liquid is stationary, the liquid is still. Still, this will happen over many hours. And what actually causes this if you recall, your earlier physics is a thermal motion of molecules, as long as there is a certain temperature, there is motion of molecules. And there is the water molecules jiggling, hitting against each other and so on so forth, various different motions of molecules. They are interacting with these molecules that ink molecules and as a result of these interactions as a result of these thermal motions. The ink molecules get spread uniformly throughout the liquid. So, the net effect is the movement of ink molecules from a region of high concentration to others of lower concentration, initially, there was no ink here, the ink concentration and the other spaces was 0.

Here it was the ink concentration in the drop that we let out. So, this is at a higher concentration at the point of its release compared to the remaining regions and the thermal motion effectively, although it is all random in all directions. Effectively, it has cost the movement flow of ink molecules from a region of high concentration to the region of lower concentrations. Till ultimately the concentrations in all parts of interest become equal. This is a very classic experiment, there must be videos that you can watch of this experiment.



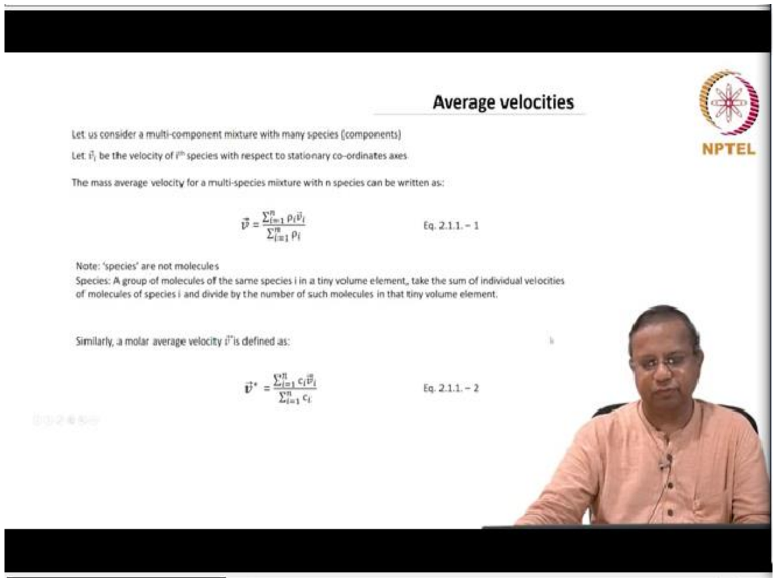
Look at that. So, what causes this flux I think I have given you the answer already a certain driving force you can look at this as a driving force. What is the driving force for mass flux, a difference in concentration over a distance right, and that is actually called the concentration gradient. The variation in concentration over a certain distance is the concentration gradient.

Strictly speaking, it is the difference in chemical potential or the chemical potential gradient, if you recall your thermodynamics and, the chemical potential gradient is the driving force for mass flux. But if it is within the same phase and concentration is a very good approximation for chemical potential and therefore, if it is within the same phase, we can replace the chemical potential with concentration and will be perfectly fine. Across phases is a different story. But within the same phase between by same phase I mean, only a liquid phase, only a gas phase and so on so forth. However, if you go from a liquid phase to a gas phase or from a gas phase to a liquid phase, inter phase transport, then the picture becomes very different you cannot use concentrations, you know the reason from thermodynamics.

It is only the equality and chemical potential that determines equilibrium, if you recall your thermodynamics. So, the difference in chemical equilibrium is chemical potential, which is the actual driving force for this, but we do not have to be so strict because the concentration works especially within the same phase. Note this the concentration difference over a distance is primarily or firstly linked to mass flux.

Let me repeat this, the concentration difference or distances primarily are firstly linked to mass flux. And there could be many driving forces that cause a much higher flux. For example, if we did the same experiment but we drop the liquid and after dropping the ink. If we stirred the container, the distribution of ink molecules, across the liquid would have been much faster. We all know this, you take, let us say, if you take sugar with your tea or coffee. If you add sugar and let it be aside for some time, it is going to take a long time for the sugar to diffuse into liquid uniformly. So, that you feel the sweetness when you drink it. However, all that we usually do is we add sugar, we take a spoon and we stir it. This is providing another driving force, this is not the concentration difference with distance, this is another driving force which we will look at later.

This driving force causes much faster flux. However, we do not consider it to be primarily linked to the mass flux and therefore this is a different driving force, there could be many driving forces that cause mass flux. However, let us first look at the primary driving force that causes mass flux and that is going to be a theme throughout the course. We are going to see the effect of the primary driving forces first on individual fluxes, mass first and momentum, then energy, then charge. And then, in the last chapter, we look at the simultaneous contribution of different driving forces to the same flux or different fluxes. So, that is going to be the theme for this course.



Now let us start the nitty gritty details, you need a certain framework to understand this, so that is what I am going to give you first. And then if you stay with it for something, then you will see how it applies to get useful information to draw insights which will be helpful in design, operation and to begin with analysis then design, then operation and so on so forth. So, let us begin. First, you need to know something about average velocities.

That is something that you already know, but let us look at it in a way that would be helpful to us. Let us consider a multi component mixture with many species with many components. Let v_i be the velocity of the ith species with respect to stationary coordinate axes. Most of our discussion will be with respect to stationary coordinate axes, I will mention that sometimes I may not mention it many times.

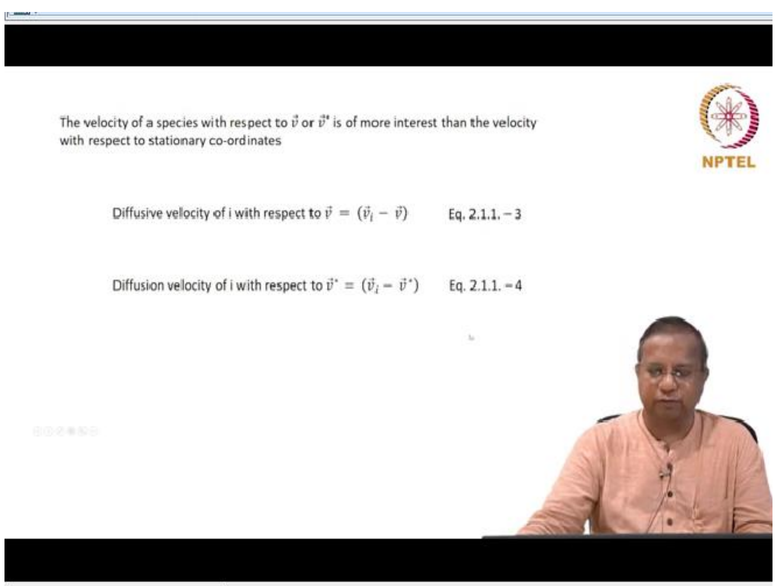
So v_i is the velocity of the ith species. The mass average velocity for a multi species mixture, with n species can be written as by the standard definition of average. And this is the average velocity we had $\vec{v}$. This equals the product of the density times the velocity of each species i and then sum over all those products. Divide the entire sum by the sum of all the densities. That is the average velocity $\vec{v}$.

$$\bar{v} = \frac{\sum_{i=1}^{n} \rho_i \bar{v}_i}{\sum_{i=1}^{n} \rho_i} \qquad 2.1.1\text{-}1$$

So, you are multiplying the density by the velocity, this is the weighting factor here, you are trying to get a certain average here. So, the weighting factor times the individual velocities, divided by the sum of the weighting factors, the standard definition of the average. Let us call this equation, 2.1.1 - 1 to be consistent with the textbook.

Species are not molecules, species is a concept, it is something like a neighborhood concept in mathematics. It is small enough to be considered some sort of representation, but it is and large enough so that the individual molecule level aspects are not taken into account here. More specifically species is a group of molecules with the same species i in a tiny volume element. And we take the sum of individual velocities of molecules or species i and divide by the number of such molecules in that tiny volume element. So, that is what gives us the average of the species, it is not with respect to individual molecules by orders with respect to the species. Similarly, the molar average multiplied by the mass density gives the mass average. Here the molar average which we are going to represent by $\overrightarrow{v *}$ equals the weighting factor. Here is concentration, c_i times v_i. Take the sum over all species divided by the sum over all species c_i. So, this is a straightforward definition, recall from your earlier courses, earlier experiences and so on. So, we will visit this again and again we will write various things in terms of this, the very fundamental formulation that each species has a certain velocity at a microscopic level. And we are working from that place forward. So, it is very fundamental. We will call this equation 2.1.1 - 2.

$$\bar{v}= \frac{\sum_{i=1}^{n} c_i \bar{v_i}}{\sum_{i=1}^{n} c_i} \qquad 2.1.1\text{-}2$$



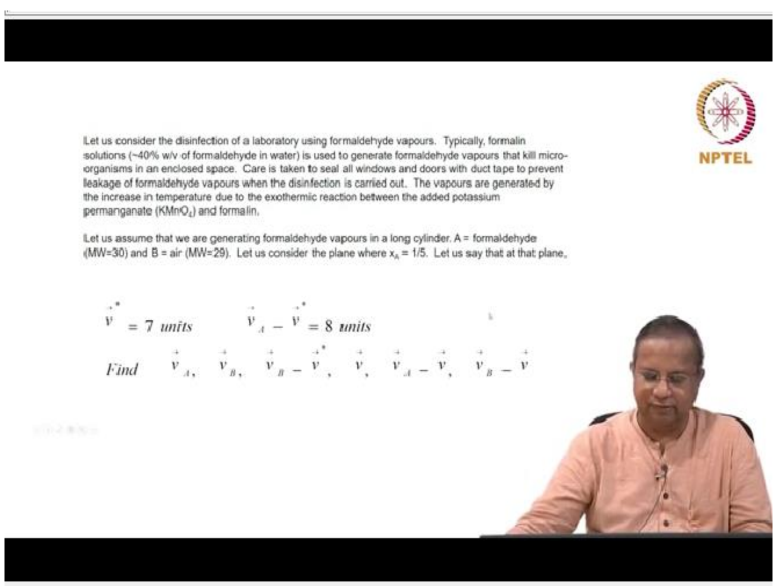
The velocity of a species i with respect to v(mass average) or v*(molar average) is of more interest than the velocity with respect to spatial coordinates, if you are looking at a mixture, you would like to know how one species is comparing with other species in terms of its movement right, you are usually more interested in that, then its motion with respect to a certain fixed stationary or fixed set of coordinates.

And therefore, the comparison is more relevant or more useful, that comparison is given in terms of diffusive velocity of i, with respect to v. So, you take v_i of any species, subtract the mass average velocity. This will give you something called the diffusive velocity of i, with respect to v, v_i-v 2.1.1 - 3 and you could also have the other one, the diffusion velocity of i with respect to molar average velocity, v*, v_i – v*, 2.1.1 - 4.

Diffusive velocity with respect to mass average velocity: $\vec{v_i} - \vec{v}$ 2.1.1-3

Diffusive velocity with respect to molar average velocity: $\vec{v_i} - \overrightarrow{v*}$ 2.1.1-4

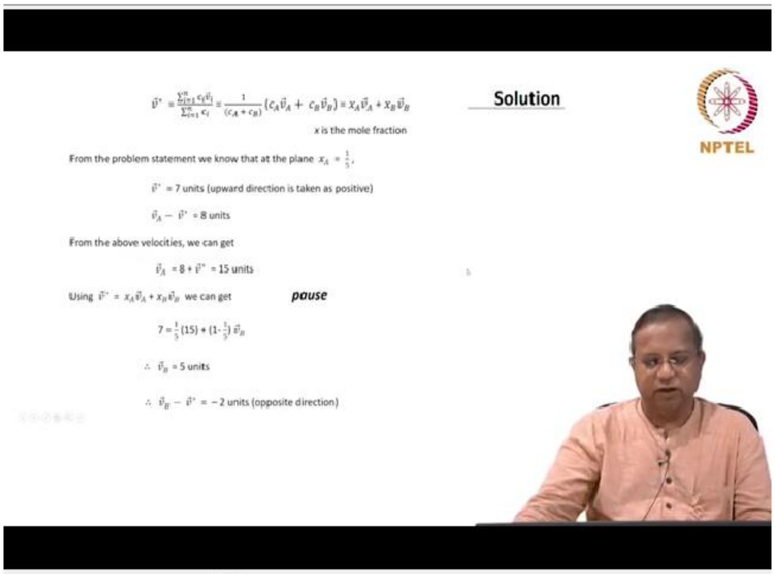
This is pretty much what we need to be able to start making fundamental sense of movement in a system of interest to us. We have just looked at averages, mass average velocity, molar average velocity of a certain species i. And then we also saw the difference that is the diffusive velocity of i with respect to v or diffusion velocity of i with respect to v*. These are the only definitions that we have seen. So, let us start using this so that we become more comfortable in its use.



To do that, let us look at a problem. Let us consider the disinfection of a lab using formaldehyde vapors. This is typically done in any lab. Typically formalin solutions, about 40% weight per volume of formaldehyde and water is used to generate formaldehyde vapors that kill microorganisms in an enclosed space, standard laboratory disinfection mechanism, care is taken to seal all windows and doors with duct tape to prevent leakage of formaldehyde vapors when the disinfection is carried out. The lab is closed, we will not or want not to enter, then the doors and windows are all completely sealed, gas sealed and then this is done, the vapors are generated by the increase in temperature, due to the exothermic reaction between the added potassium permanganate $KMnO_4$ formalin, which is the 40% vapor volume solution of formaldehyde and water.

Let us assume that we are generating formaldehyde vapors in a long cylinder for understanding purposes. Let us say A is formaldehyde with a molecular mass of 30, and B is air. Let us consider the plane in the long cylinder, the various planes in the long cylinder, where the mole fraction of formaldehyde(x_A) is 0.2 (one fifth). And let us say at that plane, we know molar average velocity, $\overrightarrow{v*}$is 7 units, this diffusion velocity v_A - v* is 8 units. And it asked to find v_A, v_B, v_B – v*, v, v_A - v* ,v_A – v, v_B - v, the last two are with respect to mass average velocities. $\overrightarrow{v*}$is 7 units is the molar average velocity that is given here and you have diffusion velocity v_A - v* is 8 units, you are asked to find the others, just by using the definitions that we have so far. And this would give you a good handle on how to use the various definitions to make sense of an actual situation.

Let me give you the solution right away, probably in between the solution that can give you some time to work it out. Pretty much the first problem that rather one of the first problems in the main theme of this course. So, let me start out first.



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

Also, the mass fraction of A

$$w_A = \frac{m_A}{(m_A + m_B)} \qquad (2.1.1\text{-}6)$$

If we divide both the numerator and the denominator of the RHS of Eq. 2.1.1-6 by V, we get

$$w_A = \frac{\rho_A}{\rho_A + \rho_B} \qquad (2.1.1\text{-}7)$$

By using Eq. 2.1.1-7 in Eq. 2.1.1-5, and using a similar expression for w_B we get

$$\vec{v} = w_A \vec{v}_A + w_B \vec{v}_B \qquad (2.1.1\text{-}8)$$

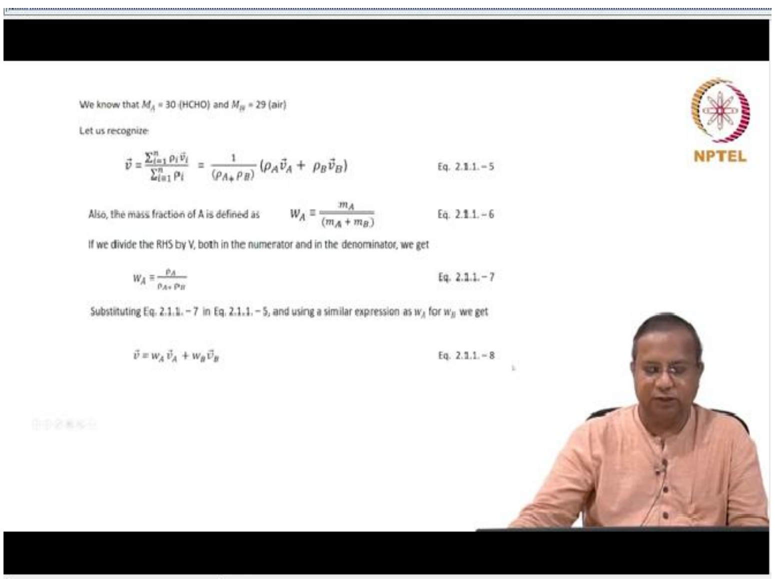
Also

$$\vec{v}^* = \frac{\sum_{i=1}^{n} c_i \vec{v}_i}{\sum_{i=1}^{n} c_i} = \frac{1}{(c_A + c_B)} (c_A \vec{v}_A + c_B \vec{v}_B) = x_A \vec{v}_A + x_B \vec{v}_B \qquad (2.1.1\text{-}9)$$

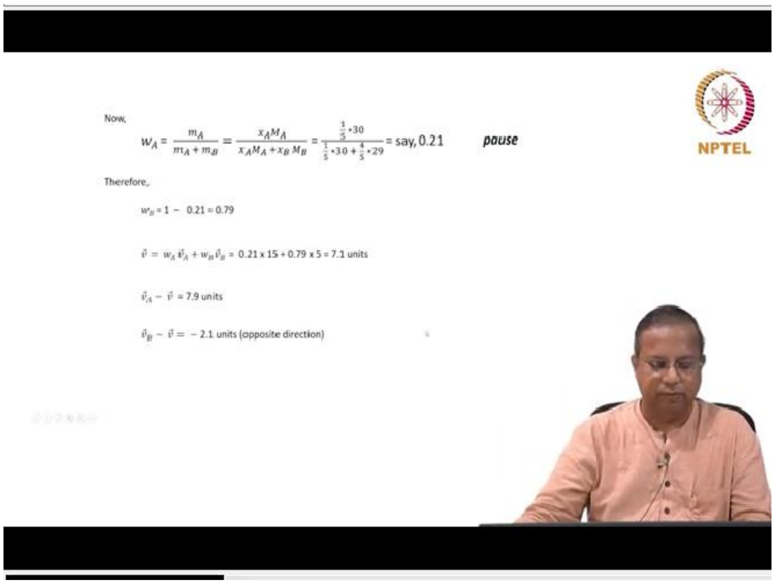
where x = mole fraction.

The molar average velocity is sum of $c_i v_i$ divided by sum of c_i. In this case you have only 2 components formaldehyde and water right. So, A is formaldehyde, B is air. We know that [1/∑ ci] times ($\sum c_i v_i$), that is the way it is written here, So, [$1/(c_A + c_B)$] times ($c_A v_A + c_B v_B$) gives $\vec{v}$. $c_A v_A + c_B v_B$ and you know that the ratio of the concentration of A species with respect to the total concentration is nothing but the mole fraction. Therefore $\frac{c_A}{c_A+c_B}$ is x_A and $\frac{c_B}{c_A+c_B}$ is x_B, we get $x_A v_A + x_B v_B$ where x is the mole fraction(moles by total moles).

For the problem statement we know that plain **x_A is 0.2(1/5).** we know $\overrightarrow{v*}$ **is 7** units, in this case we are taking the upper direction as positive and this **diffusion velocity $v_A - v^*$ is 8 units.** Again, positive here. Thus v_A is 15.Using v^* as $x_A v_A + x_B v_B$.(2.1.1-9), we know that can you substitute this and get the relevant velocity of interest here, you know v_A , x_A and x_B ($x_B = 1 - x_A$). And you can find v_B from here. Can you go ahead and do that. Also note that the concept is applicable to mass fraction ($w_B = 1 - w_A$).



I just go through it, you can work out various details. We know that the molecular mass of formaldehyde (HCHO) as you know, is M_A , is 30 HCHO you could take the atomic masses get the molecular mass and the molecular mass of air, if you take it predominantly as a mixture of oxygen and nitrogen will turn out to be around 29, M_B is 29(28.97 g/mol).



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

From $\vec{v}^* = x_A\vec{v}_A + x_B\vec{v}_B$, we get

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

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

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

Now, we know that

$$w_A = \frac{m_A}{m_A + m_B} = \frac{x_A M_A}{x_A M_A + x_B M_B} = \frac{\frac{1}{5}\times 30}{\frac{1}{5}\times 30 + \frac{4}{5}\times 29} = \text{say, } 0.21$$

Therefore

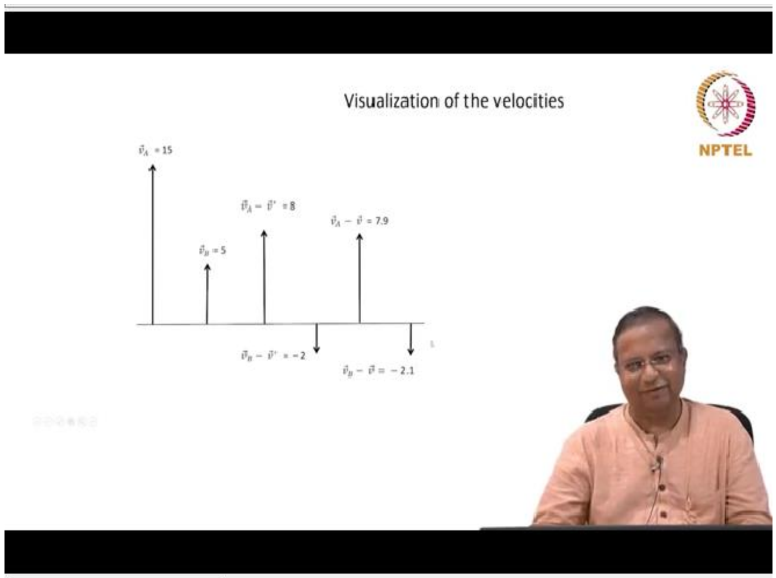
$$w_B = 1 - 0.21 = 0.79$$

$$\vec{v} = w_A\vec{v}_A + w_B\vec{v}_B = 0.21\times 15 + 0.79\times 5 = 7.1 \text{ units}$$

and

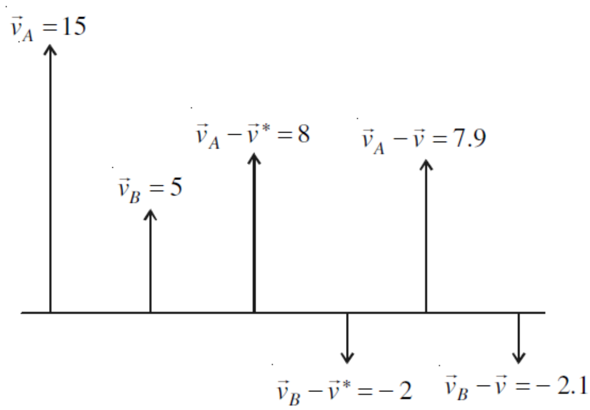
$$\vec{v}_A - \vec{v} = 7.9 \text{ units}$$

$$\vec{v}_B - \vec{v} = -\,2.1 \text{ units (opposite direction)}$$



And this is a certain visualization of these velocities, v_A = + 15, v_B was = + 5, $v_A - v^*$ = 8, $v_B - v^*$ = - 2, $v_A - v$ = 7.9, $v_B - v$ = - 2.1 or 2.1 in the other direction.

Fig. 2.1.1-2 Visualisation of the various velocities in the cylinder



So, this is what we are able to find the velocities of these species, as well as the diffusive velocities, with respect to averages. And that gives us a certain picture of the movement of molecules in that long hypothetical cylinder that we took. So, this is the starting point of building up or the building up of the formulation itself. Let us stop here. We have been at it for some time now, it is good to take a break, come back in the next class and take things forward. See you then.