

Fundamentals of Combustion
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Lecture - 17
Mass Transfer Basics - Part 02
Calculation of Diffusion Velocity

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Diffusion Velocity ✓

Dividing the equation, $\rho_A v_A = \rho V Y_A - \rho D_{AB} (dY_A/dx)$ by ρ_A , the velocity of species A is written as,

$v_A = V - \frac{\rho D_{AB} (dY_A/dx)}{\rho_A}$ or $v_A = V + v_{A,diff}$ ✓


Here, the **diffusion velocity** of species A is given as,


$v_{A,diff} = -\rho D_{AB} (dY_A/dx) / \rho_A = (-D_{AB}/Y_A) (dY_A/dx)$ ✓

In multi- dimensions, Fick's Law and diffusion velocity for a binary system are written as,

$\rho_A \vec{v}_A = \rho V \vec{Y}_A - \rho D_{AB} \vec{\nabla} Y_A$

$\vec{v}_{A,diff} = -\frac{D_{AB}}{Y_A} \vec{\nabla} Y_A$





Now we will define what is called Diffusion Velocity. We will see what is the diffusion velocity. So, take the Fick's law again $\rho_A v_A = \rho V Y_A - \rho D_{AB} (dY_A/dx)$.

Now, let us divide this equation by ρ_A , the density of the species A. So, we can write left hand side as v_A species velocity of the A and here we divide $\rho_A V$ by ρ_A . If you divide you will get just V.

So, that is the bulk velocity minus this term appears that is $\rho D_{AB} (dY_A/dx) / \rho_A$. Now, this is a species velocity v_A , V is the mixture velocity. So, this should be a velocity obviously, that velocity I call it as the diffusion velocity of species A. v_A represents this is diffusion velocity that is calculated using the product of ρD_{AB} and the concentration gradient or the mass fraction gradient divided by ρ_A . So, here this diffusion velocity can be written as $\rho D_{AB} (dY_A/dx) / \rho_A$, now the ρ / ρ_A can be written as $1/Y_A$.

So, Y_A is a mass fraction of the species A $\times dY_A/dx$ in the x direction. So, this is actually one dimensional. The diffusion velocity of species A is written as minus $(-D_{AB}/Y_A) \times dY_A/dx$.

So, you can just verify the units m^2/s for the D_{AB} , mass fraction does not have a unit. Similarly, here dY_A mass fraction does not have a unit divided and x is in m. So, m/s that will be the unit for diffusion velocity.

Species velocity can be written as sum of V + diffusion velocity. So, v_A is calculated as the mixture velocity plus the diffusion velocity, diffusion velocity in a simple way can be calculated using the concentration gradient and the binary diffusivity.

Now, in a binary mixture it is very simple to use a binary diffusivity D_{AB} like this and the gradient can be in one direction, if you want to extend this to multiple directions you have to calculate velocity which will have three components in x y and z direction. So, v_A may be diffusion velocity in the x direction.

Similarly, you can have another component say w_A diffusion in y direction. So, here the gradient will be dY_A/dy or in vector form we can write this as here.

In vector form the Fick's law itself can be written in this way, ρ_A , the density of the species A $\times v_A$, the species velocity of A and it is a vector; that means, it is resolved in three directions in a three-dimensional flow.

And ρ is the mixture density and the V vector is the mixture velocity vector $\times Y_A - \rho D_{AB} \times \nabla Y_A$ that is. So, in this way you can write and same definition you can apply and get the diffusion velocity vector of species A, $v_{A,diff} = -D_{AB} \nabla Y_A / Y_A$. So, this is a very simple way of calculating this. The main thing is we have to first calculate.

So, it is easy to calculate or measure the mixture velocity. You can solve numerically the Navier Stoke equations to get the velocity or if you want measure you can use any methodology like pitot tube or a PIV or anything to get this. Then next challenge is to get the species velocity.


So, I need species velocity considering each species in a multi component mixture, we need to conserve all the individual species. For that you have to form a governing equation which involves the species velocity.

Since we cannot measure that we have to calculate that in terms of the mixture velocity and the diffusion velocity. So, we have to calculate diffusion velocity in a particular way. For example, now in a convective term of species conservation the mixture velocity V will appear along with the diffusion velocity.

For conserving each species, we need the species velocity in the convective terms. So, in a very simple form we can write the diffusion velocity as $-D_{AB} \nabla Y_A / Y_A$ but if you see this is only for a binary mixture when there are more than two species present how are you going to do this. It can be as simple as what we have written here.

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Diffusion Velocity



The diffusion velocity discussed so far is due to ordinary mass diffusion alone. However, in real mixtures, especially in combustion, gradients due to temperature and pressure can produce species diffusion; called thermal diffusion (Soret) and pressure diffusion, respectively. In addition, unequal body forces per unit mass among the species would lead to force diffusion. The diffusional velocity combining all the above is given as,

$$\vec{v}_{A,diff} = \vec{v}_{A,diff,X} + \vec{v}_{A,diff,T} + \vec{v}_{A,diff,p} + \vec{v}_{A,diff,f}$$

The suffices X, T, p and f denote diffusion due to mass fraction gradients, temperature gradients, pressure gradients and body forces, respectively. Ordinary mass diffusion is significant in all the problems.



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Now, before going to the multi component mixture let us see some other characteristics of diffusion velocity. For diffusion velocity what we considered in the previous slide is only due to ordinary mass diffusion; that means, it has only concentration gradients. The mass fraction gradient what we have written that is only contribution that is only contributing factor there.

So, higher the concentration at one location and lower the concentration at another location and due to the concentration gradient that diffusion takes place. But please understand that this is basically due to concentration gradient, but if you take combustion reactions etcetera you will see the temperature gradients will be very high.

Since we can see that the temperature zones will be concentrated to a particular small region in the flame.

So, here the temperatures are very high within the flame zone but if you go to this direction or this direction the temperature reduces to the ambient value.

So, a large temperature gradient is seen. A huge gradient of temperature is seen in several scenarios. In a compressible reactive flow pressure gradients can also be very high, but not in normal burners and stoves. Pressure gradients are not negligible if you take say aerospace applications.

So, you can see that the pressure gradients can also be high. When the mixture comes at a very high velocity and burns and products leave at a very high velocity then the pressure gradients can also be high. So, if there are huge concentration of temperature and pressure, they will also contribute to what is called species diffusion.

If the species diffusion occurs due to temperature gradient then it is called thermal diffusion or Soret effect. If the diffusion takes place due to pressure gradient then it is called pressure diffusion. So, these are the two additional diffusion velocities which you will get.

So, one is due to the ordinary diffusion which is very common for any multi component mixture even it need not be a reactive flow normal flow but some small temperature gradient may be there. So, the temperature-based diffusion can be neglected, but the ordinary diffusion is still important there.

If its just an air flow, wherever you measure the gradient concentrations, the concentration of oxygen is only 0.21 everywhere; obviously, minor changes may be there.

Then you need not even worry about the diffusion, but on the other hand if there is a concentration gradient, say two different fluids like say oxygen and carbon dioxide mix even the temperature may be isothermal like 300 K, even in that scenario you need to add ordinary diffusion due to concentration gradient.

But the thermal based diffusion requires very high temperature gradient. Similarly, pressure diffusion requires a very high pressure gradient. Apart from this unequal body forces per unit mass, see for example, as I told you if you take say methane, methane has a molecular weight of 16 much less than an air. Air molecular weight is around 28.85.

So, hydrogen converts into water vapor and carbon converts into carbon dioxide. Water vapor's molecular weight is 18, but CO₂'s molecular weight is 44. So, you can see the species of different molecular weights are available. So, unequal body forces can be created. Again, this is not in every scenario.

In some scenario unequal body forces can prevail in a mixture, so, that will also lead to what is called body force based diffusion. So, this body force based diffusion also can be added.

Now, this means the diffusion velocity what we are going to calculate here will be dependent on the diffusion velocity due to concentration gradient, where I put suffix x to represent that this is the concentration gradient based diffusion velocity.

Similarly, diffusion velocity due to Soret effect or the thermal diffusion where I put a T in the suffix to represent that is due to temperature gradient. Similarly, diffusion velocity due to pressure gradient p, I am putting here. Similarly, due to body force gradient unequal body forces we can have diffusion velocity.


In several scenarios the last two terms will be very low and you can neglect it, but in very low speed high diffusion type of scenarios the second term, that is the Soret diffusion will be very important. In all scenarios the ordinary mass diffusion is significant.

So, the diffusion velocity is contributed by ordinary diffusion due to mass fraction gradient, thermal diffusion due to temperature gradient, pressure diffusion due to pressure gradient and body force due to the unequal body forces per unit mass.

So, how to calculate this is very important. We have already seen a simple way to calculate the ordinary diffusion that is minus $-D_{AB}/Y_A \times$ mass fraction gradient. So, how to calculate this we will see now.

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Multicomponent Diffusion



For a mixture with more than 2 components, a **multicomponent formulation** is required. The diffusion velocity of each species is calculated by solving a set of equations called **Stefan-Maxwell equations**. Here, D_T is thermal diffusion coefficient in kg/m-s

$$\vec{v}X_i = \sum_{j=1}^N \left(\frac{X_i X_j}{D_{ij}} \right) (\vec{v}_{j,diff} - \vec{v}_{i,diff}) + (Y_i - X_i) \left(\frac{\vec{v}p}{p} \right) + \frac{\rho}{p} \sum_{j=1}^N Y_j Y_j (\vec{f}_i - \vec{f}_j)$$


$$+ \sum_{j=1}^N \left(\frac{X_i X_j}{\rho D_{ij}} \right) \left(\frac{D_{T,j}}{Y_j} - \frac{D_{T,i}}{Y_i} \right) \left(\frac{\vec{v}T}{T} \right)$$

Binary diffusion coefficient

D_T ← thermal diffusion coefficient

In right side, first term involves **ordinary diffusion**, second and third terms consider **pressure and body forces based diffusion** and final term is **Soret diffusion**. This is a thorough approach that involves lot of computations, especially, when the number of species are more.

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Now, we will add the complexity of more than two species being present. So, here we have seen the complexity of the diffusion velocity which is not only due to ordinary diffusion but temperature gradient, pressure gradient and body force gradient can also give rise to this diffusion velocity. So, we have to add up all these to get the net diffusion velocity of species A and that should be added to the mixture velocity to get the species velocity of A.

Now, let us consider the multi component formulation for the mixture with more than two component, it will work for two components also, but we will consider more than

two components here. Now the diffusion velocity of each species is calculated by solving not one but a set of equations and this is called Stefan Maxwell equation.

When you want to calculate diffusion velocity, we have to solve a set of equations. So, this is the gradient of mole fraction of every species. If there are N species, then there will be N reactions like this. Set of these reactions will consist of N equations for N species.

So, gradient of mole fraction will be equal to, there are four terms here the first term is due to the ordinary diffusion of any two species. So, we are trying to solve for the i^{th} species here. So, I have to loop over all the species.

So, j equal to 1. Here, N is the total number of species in the mixture. So, j equal to 1 to N . $X_i X_j / D_{ij}$, so, D_{ij} is the binary diffusivity of the pair ij . This is the fundamental property of any two species i with j . So, that is what is substituted here.

And we have v_j and v_a . So, now, you have to solve this. Let us assume you are only solving the ordinary diffusion term. Term 1 alone will be present and other terms need not be there. So, you have to solve N equations to get the velocities. Now, you can solve this together to find the total velocity.

Now, the IInd term here is the pressure gradient based diffusion. So, you can see this ∇p , the pressure gradient term here and this is the mass fraction and mole fraction here, so, this term is solved. So, just the pressure gradient you can use this. The IIIrd term here is the body forces f vector suffix i , this is the body force for the species i .

Now, please see that if these unequal body forces are there then this term will be significant. $\bar{f}_i - \bar{f}_j$ will be significant; however, if the body forces are not so high then this term will be negligible. So, the total term IIIrd term will be out. In several cases the IIIrd term will not be useful similarly the pressure gradients are also not so large. So, that is also going to be negligible.

Coming to the IVth term, here the IVth term this is the Soret effect or the thermal diffusion effect where the temperature gradient is going to be the driving force. We have used the binary diffusivity in the Ist term, ordinary diffusion, here we are going to use D_T which is nothing but the thermal diffusion coefficient.

So, this is the thermal diffusion coefficient and it has a unit of kg/ms . Again, you have to use some correlations and its not so easy to really get the characteristic value of D_T for any species i and j . Please understand based upon the species you have to calculate the this.

So, this is a very involved set of equations. Very involved set of equations and it needs lot of computations to calculate the diffusion velocities. In several cases as I told you, IInd and IIIrd term are not going to be important. They are not significant at all. For example, if the temperature gradients are not so, high.

When you are dealing with the mixture, for example, lean mixture, then the maximum temperature is around 1300°C to 1400°C something like that. The temperature gradients are not so high. In such a condition this IVth term will also drop out. But anyway only with the Ist term, this involves N equations to be solved and this is not going to be practically possible.

If you are modeling a very small flame this calculation can be done, but if you have a huge combustion chamber where you have to do this calculation it is going to be very costly. So, it will be very involved calculation for us solving n equations of this Stefan Maxwell set of equations to get the diffusion velocities.

However, when you once you get this diffusion velocity for all the species then you can add it to the mixture velocity at any location and get the species velocity at that location. So, this is very important.

So, multi component diffusion here we are trying to resolve all the diffusion due to concentration gradient Ist term then due to the pressure gradient IInd term, due to the body force gradient IIIrd term (the unequal body forces), then the IVth one is the thermal or Soret effect. (Refer Slide Time: 19:48)

Multicomponent Diffusion



In many applications, diffusion due to gradients of pressure and body forces is negligible. A **simplified approach** of determining the diffusion velocity due to ordinary and thermal diffusion is given as follows.

First, a **diffusion coefficient for a species to diffuse into the mixture, D_{im}** using binary diffusivity (D_{ij}), and then the diffusion velocity are determined as,

$$D_{im} = \frac{(1 - X_i)}{\sum_j \left(\frac{X_j}{D_{ij}} \right)}$$

Binary diffusivities & X_j

$$\vec{v}_{i,diff} = - \frac{D_{im}}{Y_i} \nabla Y_i$$

Thermal diffusion velocity is calculated as, $\vec{v}_{i,diff,T} = - \frac{D_{T,i}}{\rho Y_i T} \nabla T$



So, as I told you in many applications, the gradients in pressure and the body forces are negligible. So, the second and third term are negligible. Now, it is very costly for us to

do Stefan Maxwell equation for all the things. If you solve this set of Stefan Maxwell equation then you are solving what is called full multi component diffusion.

So, when you numerically solve any flame, and if you incorporate the solution of Stefan Maxwell equation in that, then that approach is called full multi component diffusion approach. But it is not easy to do it for all the problems. For some set of problems its fine, but not for all the problems.

So, we need some simplified approach. What is the simplified approach? here what we are trying to say is instead of calculating the diffusion velocity directly for the i^{th} species, I will only consider a binary type of scenario here.

If i is the first species then all other species in the mixture other than the i will be the second species. So, let us consider only a binary type of species here species i isolated out all other species except the i constituting a second species or bulk species. Binary diffusion coefficient is now defined as $D_{i,m}$ how the species i is going to diffuse into the mixture. So, that is calculated by a simple algebraic relationship given here.

$D_{i,m}$ is the rate at which i goes into the mixture, I do not see individually i going to j . I am saying the rate at which i diffuses into the mixture. So, $D_{i,m}$ is calculated using this relationship $(1-X_i)/\sum X_i/D_{ij}$; now here this D_{ij} is nothing but the binary diffusivity of a pair of species i and j .

Now, when j varies here it should not be equal to i you have to exclude the i here because what happens if $j = i$ then D_{ii} will come and that will be equal to 0. So, this denominator will be 1 by 0 it will be infinity. We will not be able to solve this.

So, excluding j when it becomes i we have to sum up for all other species. That is, I am trying to keep all other species as a bulk species and get the diffusion coefficient of the i to the mixture. So, when you calculate $D_{i,m}$ like this then the species velocity can be calculated in a simple way.

So, instead of solving N equations as a gradient of X_i equations I am just solving algebraic equation like this. So, at a given point we know the mole fractions of all the species. I can take any two pair of species, calculate D_{ij} and finish this calculation $D_{i,m}$.

Once I know the value of $D_{i,m}$ then I substitute here $v_{i,diff}$. This is due to the ordinary diffusion and will be equal to $-D_{im}/Y_i \times \nabla Y_i$. Now, instead ∇Y_i I can put gradient of Y_A . Similarly, what I am putting here is $-D_{im}$ which is calculated using this.

I am taking the help of binary diffusivities of any two species and that is summed up for all the species. So, I can use this as a diffusion coefficient for the i^{th} species going into

the mixture. So, this is the way you calculate the diffusion velocity of the particular species i .

Now thermal diffusion velocity can be calculated once you know $D_{T,i}$. Thermal diffusion velocity $v_{i,diff,T}$ can be calculated as $-D_{T,i}/\rho Y_i \times (1/T) \nabla T$.

Now, the total velocity will be sum of these two, ordinary diffusion + the Soret diffusion. That will be the total diffusion velocity that you add to the mixture velocity to calculate the species velocity of i . So, this is a simplified approach. You do not need to solve this N equations like this to get the value of V_i .

Individually, first you calculate using an algebraic equation for $D_{i,m}$, the diffusion coefficient of the i^{th} species into the mixture and based upon that you calculate the diffusion velocity $-(D_{im}/Y_i) \times \nabla Y_i$ and thermal diffusion velocity is calculated using the thermal diffusion coefficient $D_{T,i}$.

So, $(D_{T,i}/\rho Y_i) \times (1/T) \times \nabla T$. So, this is the way you calculate and add these two to get the net diffusion velocity of species i at a particular point that add to that the mixture velocity you get the species velocity of i at the particular point.



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Steady Evaporation – Stefan Problem ✓

Consider a liquid A maintained at a fixed height in a glass cylinder, on top of which two gases A and B flow across

Gases A and B
 $x = L$
 $Y_{A,\infty}$ at $x = L$
 $Y_{A,i}$ at interface
 $x = 0$
 Liquid A

Concentration of gas A flowing across is less than that at interface.
 Following assumptions are made:
Steady state exists ✓
Liquid level is maintained constant ✓
Gas B is insoluble in liquid A ✓
Stagnant layer of B is in the column between $x = 0$ and $x = L$ ✓

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Now, let us consider the first example. Till now we are only dealing with the gaseous mixture, that is within the gaseous mixture how the diffusion can take place because of the gradients. For example, if air is flowing in a horizontal duct and as a cross flow a fuel can be injected.

So, you can see how the fuel and air mixes. Initially, at the point of injection the fuel concentration will be higher and it is first partially carried by the air and it also diffuses towards the direction where its concentration is low. In several scenarios you can see that

when the convection is higher and higher, then diffusion contribution will be lower because the convection will suppress the diffusion.

For example, if diffusion is trying to transport the species in the direction opposite to the convection based upon the strength of the convection, this will be nullified.

Now let us take a problem where you have a liquid phase also. So, liquid phase and how the evaporation is done and how we are going to analyze the evaporation of a liquid surface.

For that we will consider what is called a Stefan problem. Stefan problem is nothing, but where you have a test tube as this, a cylindrical vessel, a test tube in which a liquid is present. Liquid A is present and please understand that this liquid is also fed at a very slow rate which is the rate at which the evaporation of liquid A takes place across the interface.

So, evaporation takes place and this is the interface $x = 0$. Across the interface the liquid is converted into vapor and the vapor escape to the gas phase. So, this is the gas phase and this is a liquid phase. So, vapors go to the gas phase.

Similarly, condensation can occur. So, the gas which has a vapor A can condense. Now, you are seeing the evaporation problem. That means, this temperature here, say T_{∞} , is sufficient enough to provide the energy to evaporate the liquid.

One more important point is when there is evaporation which is taking place and if you do not supply the fuel, then the surface of the interface will regress; that means, the interface will come down, but what we are trying to do here is a fixed interface problem; that means, the rate at which the fuel is evaporating, I try to supply liquid A slowly so that the level is maintained at $x = 0$, liquid level is maintained at $x = 0$ which is the interface point.

Now, consider liquid A maintained at a fixed height in a glass cylinder or a test tube. On top of this two gases A and B flow. Please understand that gas A is a condensable gas. Gas B is like nitrogen, a non condensable gas which flow across at normal temperature and pressure.

Now, concentration of gas A flowing across is less than that of interface; that means, $Y_{A,i}$ is higher and $Y_{A,\infty}$ is lower. That will only drive the fluid from this interface to the ambient by diffusion. So, that concentration gradient prevails in the same direction as the convection. So, how convection comes here?

There is a liquid in a tube and there is a flow which is the slow flow of gases A and B which is in the horizontal direction. But what we are interested in is the transport in the x

direction. So, this is the direction I want to resolve and then put. There is no convection initially present. So, how convection comes in that is what we are going to see.

So, concentration of gas A or vapor A flowing across is less than that of the interface that will drive the A from the interface towards the ambient by diffusion. Now, following assumptions are invoked. First, steady state exists. How steady state can exist? If there is no supply of liquid then the liquid surface will regress it will fall down slowly as the liquid is evaporated.

So, that means, steady state cannot be there. With the function of time the level of the liquid will change. That means, steady state cannot be prevailed. Now, you can ask one question. There is a constant evaporation so how can you call it as steady state with time you know the evaporation can change? The answer is, the rate of evaporation need not change with time that is what the steady state assumption means here.

That means, evaporation takes place slowly and the liquid is also fed to maintain the level constant here. If the level is maintained constant here then the diffusion scale here 0 to L, that is also maintained constant. So, we can get steady state evaporation.

So, you can say its a quasi-steady; that means dynamic evaporation is also happening. That is dynamically you can see that there are some transfer phenomena happening in the x direction, but it is happening at a steady rate.

So, steady state exists that is the first assumption made. Liquid level is maintained constant by supplying the liquid A at the rate at which it evaporates. So, that is the way we maintain the steady state evaporation.

If we do not do this then the evaporation will be unsteady. Now one more point is gas B say nitrogen or oxygen whatever. So, let us say nitrogen, is insoluble in liquid A. Liquid A may be a fuel say methanol or ethanol and liquid A will form its vapor that is ethanol vapor or methanol vapor will form and that will mix with the ambient gas that is say nitrogen.

In an evaporation problem let us consider nitrogen we do not even need to go to the oxygen scenario where a combustion can take place. Now what this assumption means can nitrogen dissolve in ethanol or methanol?

Yes, it can happen when the pressures are very high. For example, if you go to say 10 bar, 12 bar, 15 bar and 20 bar etcetera based upon the critical pressure there is a there is a good chance that the gas in the ambient can dissolve into the liquid.

And it can also vaporize and come out along with the vapor A so that means, this dissolution is possible. Dissolving the gas into liquid is possible at higher pressures, but

we are not concentrating on that scenario and this is a very simple open atmospheric pressure problem. So, gas B is considered as insoluble in liquid A that is important assumption made.

This will keep the liquid phase as single component. If gas B dissolves into the liquid, then it will become a two component in the liquid phase. Then the fourth one, also we will see the stagnant layer of B present in the column. What do you mean by stagnant layer of B?

So, predominant flow of B is in the other direction. This is the x-direction the vertical direction is x here. So, we can say the vertical direction is x and the horizontal direction is y. So, that is the frame here. In this when I say stagnant layer of B in the column this $x = 0$ to L ; that means there is no velocity for B in this column.

So, only by diffusion B comes down into this. So, obviously, in a binary mixture like this $1 - Y_A = Y_B$. So, you can very easily calculate Y_B .

Since Y_B which is present in this column between $x = 0$ to $x = L$ that means that layer is going to be a stagnant layer which has transported B due to diffusion. So, this is the fourth assumption made. So, how will you solve this problem?