Heat and Mass Transfer Prof. U.N. Gaitonde Department of Mechanical Engineering Indian Institute of Technology, Bombay Lecture No. 33 Introduction to Mass Transfer-1

Welcome back. We will now move over to the ninth and final part on this series of lectures on heat and mass transfer.

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This section is called mass transfer. In the next few lectures, we will undertake a basic introductory study of the phenomena of mass transfer.

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We will notice that there is a significant extent of similarity between the processes of heat transfer and those of mass transfer. Conduction has an analogy in diffusion, heat conduction has analogy in convective mass transfer. Because of the analogy we will find that many equations, relations, correlations are very similar in structure and we should know that heat and mass transfer occur simultaneously in many important situations. For example, clothes hang out to dry in the sun; the process of drying is a process of combined heat and mass transfer. What are we going to study in these few lectures on mass transfer?

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First, a basic law pertaining to mass transfer is the Fick's law of diffusion. We will look at it in some detail, then we will look at some one dimensional problems in a stationary medium followed by mass transfer in a moving medium, then we will look at convective mass transferring. Particularly, we would study the analogy between heat transfer and mass transfer and finally we will spend some time on simultaneous heat and mass transfer - situations in which we have to consider heat transfer as well as mass transfer occurring together. Let us begin our study of mass transfer by looking at the Fick's law of diffusion.

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The Fick's law of diffusion is analogous to Fourier's law of heat conduction. One can say that the Fourier's law of heat conduction represents or models the diffusion of heat through a material medium. The Fick's law considers diffusion of mass through a material medium. The Fick's law of diffusion is valid for gas mixtures and our initial illustrations would essentially be on gas mixtures; it is also valid for liquid solutions and solid solutions. We should notice that the Fick's law of diffusion is an empirical law and is based on experimental evidence, similar to Fourier's law which is an empirical law and is based on experimental evidence.

Suppose we have a confined gas and in which there is a mixture of gases. Let us say that we have a concentration of some component A; so we can say this is concentration of component A. A is more densely packed on the left hand side, is more lightly packed on the right hand side. So the A has a higher concentration near this zone A, has a lower concentration at this thing because of this concentration gradient decrease in concentration as we move to the right. Let us say this is direction x, there is a flux or a flow at the microscopic level of component of A. This is known as the diffusion of A; Fick's law relates the concentration gradient to the rate of diffusion of A.

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Let us consider a mixture of 2 gases A and B and let us consider gas A diffusing into gas B. The Fick's law of diffusion says that the mass flux of gas A in a particular direction A is proportional to the density of the mixture and the concentration gradient in that direction. n is the direction variable and w_a is the mass fraction of component A. So this is the mass flux of A component; this A here represents area and that is why we will get a mass flux. m dot a will be the mass flow rate or diffusive flow rate, so the units of m dot a will be say kg per second, units of area are meter square. So, the units of mass flux are kg per meter square second.

On the right hand side, we have density units kg per meter cube. n is the space variable direction units meters and w_a is the mass fraction of A - it is a dimensionless number. If you want units, you can write the units as kg of A per kg of mixture. Now since we have 2 components A and B, we must know what is meant by the mixture density rho, the mass fraction of A and the mass density of A. Let us say that rho A is the mass density of A.

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Fick's law of diffusion (Contd) mass density of gas A, and If ρ_{α} mass density of gas B, then ρ_b $\rho = \rho_a + \rho_b$ and $w_a = (\rho_a/\rho)$ $W_k = (f_k/e)$

This, the units will be kg of A per meter cube of mixture. Similarly, the second component B will have a mass density of B which will be kilogram of B per meter cube of mixture and this is the gross or total density which is the sum of the densities of the component A and the component B and it will have units kg per meter cube. The mass fraction of A will be the mass density of A divided by the total density. Similarly, if you want to write down the mass fraction of b, it will be rho b divided by the total rho; this will be the mass fraction of b.

We have seen that the basic form of Fick's law of diffusion gives us a proportionality between the mass flux of A and its concentration gradient. The constant of proportionality is called the mass diffusion coefficient or the diffusion coefficient.

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It is given the symbol D for diffusion coefficient with subscripts ab; ab indicates that the mixture is made up of gases a and b or components a and b and a is diffusing into b. With this constant of proportionality, the Fick's law of diffusion looks like this. This is the mass flux of component a in direction A equals minus rho D_{ab} and the derivative partial derivative of w_a in that direction. Notice the negative sign very similar to the negative sign in the Fourier's law of heat conduction. Here we put the negative sign to indicate that when the concentration of a decreases in a particular direction, the mass flux is towards that direction.

So, just the way heat gets conducted down a temperature gradient, mass in a mixture diffuses down the concentration gradient. The mass flux is from a zone of higher concentration towards a zone of lower concentration. Notice that we have a density here and a mass fraction here and the product of density and the mass fraction would be the mass density of that particular component. So, if the density of the mixture rho is uniform - which is often the case - then we can write the Fick's law of diffusion in the slightly different form, in terms of the mass density of component a.

So, the mass flux of a in a direction n will be minus D_{ab} into partial derivative of rho a in the direction n. Notice the similarity between this and the Fourier's law of heat conduction. Suppose we select a Cartesian coordinate system; so in a Cartesian coordinate system we will have 3 directions.

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Fick's law of diffusion (Contd) In Cartesian coordinates, Fick's law can we written as: $=-\rho D_{ab}\frac{\partial w_{a}}{\partial x}$ $= -\rho D_{ab} \frac{\partial w_a}{\partial y}$ m_a $=-\rho D_{ab}\frac{\partial w_a}{\partial z}$

x, y and z and the Fick's law in each direction can be written down in terms of 3 relations - one for the x direction, onefor the y direction and one for the z direction. Notice that the diffusion coefficient for component a diffusing into a second component b is the same in the three directions. This indicates that for the purpose of writing these expressions, we have assumed that we have an isotropic mixture. We may also express Fick's law of diffusion in a vector form; then on the left hand side we will have a mass flux vector.

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This vector will have 3components - mass flux in the x direction, mass flux in the y direction and mass flux in the z direction - and on the right hand side we have density and the diffusion coefficient which are scalars and gradient of the mass fraction. The gradient of the mass fraction will be a vector and the 3 components of this vector would be partial derivative of w_a with respect to x, partial derivative of w_a with respective to y and partial derivative of w_a with respective z.

The advantage of writing any law - in Fick's law in this particular case - in vector notation is that now we can expand this vector notation in any suitable system of coordinates. We can do it in Cartesian coordinates and we will get the equations which we saw earlier. If you need to solve a problem in cylindrical polar coordinates or spherical polar coordinates, all that we have to do is express the left hand side and the right hand side in the appropriate coordinate system. The 3 components will be specific to that particular coordinate system and we will get the expressions for Fick's law in that particular coordinate system. In fact, you should notice that the expressions are very similar to the expressions for Fourier's law of heat conduction.

So you have, if you have a form of Fourier's law of heat conduction for a particular coordinate system, by analogy you can write, fix law of diffusion in that particular coordinate system. Quite often, we express the composition in terms of mole fraction and molar density.

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So, if the concentration of gas A is expressed in its mole fraction x_a or molar density c_a , then we can express Fick's law in terms of these. This will be now molar flux of component A; this will be kg mole of A per meter square per second. On the right hand side, c is the molar density of the mixture that is kg moles per meter cube, n is the direction, c_a is the molar density of component A - that will be kg mole of A per meter cube - and x_a is the mole fraction of A, that would be kg mole of A per kg mole of mixture. And notice that D_{ab} - the diffusion coefficient - will have the units meter square per second; whichever form of Fick's law we use the diffusion coefficient will have, diffusivity will have the units meter square per second.

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Again, continuing with the molar density from if c_a is the molar density of gas A and and c_b is the molar density of gas B. Again, units will be kg mole of A per meter cube of mixture and c_b will be kg mole of B per meter cube of mixture, then the total molar density is c_a plus c_b and the mole fraction of A will be c_a divided by c. And as in case of the mass fraction base formulation, if we find that the molar density of a mixture is uniform, then we can write Fick's law in a slightly simpler form in terms of the molar density. Again here, the units on the left hand side would be kg mole of A per meter square second and on the right hand side this will be kg mole of A per meter cube. n will be in meters and D will be in meter square per second. Mole fractions and mass fractions are applicable for any mixtures. However, quite often, when the mixture is a gas we tend to work in terms of partial pressures and quite often a gas mixture is made of components which obey the ideal gas law.

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Fick's law of diffusion (Contd) If the gas mixture is made of components which obey the ideal gas law, then in terms of the partial pressure of component A, p_a , we have: $\left(\frac{\dot{N}_a}{A}\right)_- = -\frac{p}{RT}D_{ab}\frac{\partial (p_a/p)}{\partial n}$ $\left(\frac{\dot{N}_a}{A}\right) = -D_{ab} \frac{\partial (p_a/\bar{R}T)}{\partial n}$ and

When each component obeys the ideal gas law, then we can express Fick's law in terms of the partial pressure of a component. For example, here we have the molar flux of component A expressed in terms of the mixture pressure or system pressure divided by RT which will give us the molar density rho D_{ab} and here the mole fraction will be the partial pressure of component a divided by the total pressure of the mixture. And by simple algebra, we can write this as minus the diffusion coefficient into d by dn partial derivative in direction n of p_a by R bar T where R is the gas constant specific to that particular gas.

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All this while we have looked at component A but if the concentration of the density of component A is changing in the direction n, that of component B will also be changing in the direction n and using Fick's law we can write an expression for the diffusion of component B into component A. This will be the mass flux of component B in direction n and using Fick's law it will be minus rho into D_{ba} into partial derivative of the mass fraction of B in the direction n. Notice that this is now D_{ba} because we are considering the diffusion of B into A. So far we have had D_{ab} which was the diffusion diffusivity for component A diffusing into B.

We have so far considered only 2 components A and B but Fick's law doesn't restrict itself to 2 component situations. It is applicable to multi component gas mixtures also; not only that, it is also applicable to liquid solutions and solid solutions – a solid diffusing into a liquid or a gas diffusing through a liquid, one liquid diffusing through another liquid or a solid a liquid or a gas diffusing through a solid. For example, hydrogen or helium diffusing through a metal sheet or through a rubber hose - Fick's law is applicable even in these cases.

Let us now look at the diffusion coefficients; there are hand books and reference books in which you will find values of diffusion coefficients, tabulated for a large number of cases.

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This is an illustrative table tabulating diffusion coefficient of some gases in air at 1 atmospheric total pressure and 25 degrees C. Diffusion coefficients are reasonably significant functions of both pressure as well as temperature so whenever you read off a value of diffusion coefficient, note down the pressure and the temperature at which it is tabulated. The values of the diffusion coefficients are small; meter square per second is a large unit. Typically, the values of diffusion coefficients are of the order of 10 raise to minus 5 minus 6 or still smaller in meter square per second so the value of diffusion coefficient multiplied by 10 raise to 5 is tabulated here for ammonia, carbon dioxide, hydrogen naphthalene, nitrogen oxide and oxygen. And you will notice that all the values are of the order of 1 to 4 into 10 raise to minus 5 meter square per second.

So, the component A, here is this component B, here is air and the total pressure of the mixture is 1 atmosphere and the temperature is 25 degrees C. One small thing to notice here is the general trend that lighter gases like hydrogen tend to have a higher diffusion coefficient and heavier gases or heavier vapors like naphthalene tend to have a lower diffusion coefficient; that is the general trend. Here, we see the variation of diffusion coefficient of water vapor in air with temperature.

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The total pressure remains 1 atmosphere but the temperature goes from 200 to 400 degrees C in some steps and you will notice that the diffusion coefficient increases; actually it more than doubles when the temperature goes from 200 Kelvin to 400 Kelvin. It is a monotonic increase in the diffusion coefficient; this is the general trend for diffusion coefficients of gases. Quite often, we need to obtain a diffusion coefficient at a pressure and temperature slightly different from that tabulated and quite often, more often we need to interpolate between tabulated values of pressure or tabulated values of temperature for a gas or a vapor diffusing through a gaseous medium.

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Diffusion coefficient (Contd) For a gas or a vapour, diffusing through a gaseous medium, the diffusion coefficient increases with temperature, but decreases as the pressure increases. In many such cases, over a small range of T and p , we have $D_{ab} \propto \frac{1}{p}$ where n is a number between 1.5 and 2.

The diffusion coefficient increases as the temperature increases as we have seen for water vapor in the previous table and the diffusion coefficient decreases if the pressure increases so there is some sort of a direct relation to temperature but an inverse relation to pressure and over a reasonably small range of pressure and temperature the diffusion coefficient of a gas A in gaseous mixture of A and B or even a multi component mixture can be represented as proportional to temperature raise to n divided by p where n is a number less that 2 usually between 1.5 and 2. So that is why you will notice that as temperature increased by a factor of 2 for water vapor from 200 Kelvin to400 Kelvin, the diffusion coefficient increase from 2.12 10 raise to 5 to 4.61 10 raise to5, a factor of more than two. That is why this exponent n here is a number greater than 1 but less than 2 and is typically around 1.5. This proportionality can be used to interpolate or slightly extrapolate the data for diffusion coefficient.

Now after this discussion on Fick's law and something about the diffusion coefficient, we will look at the next topic which is the steady state mass diffusion in a stationary medium. We are going to look at some simple problems during this set of lectures.

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Here we will look at a typical problem; the statement of typical problem has the following situation. We are going to look at steady state diffusion of a gas through a stationary large isothermal slab of width B. The slab may not be a physical solid slab; it could be a liquid layer, it could be a layer of a gas but we will use the generic word slab meaning a region of uniform thickness in large dimensions in the other directions. The mass fraction of the gas on the 2 faces of the slab is different - w_{a1} and w_{a2} . Let us sketch the situation; we are considering diffusion through a slab.

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Let us say we have slab of width b - a plane parallel slab; it is very large in this direction, also in that direction. So, if this is the x direction, it is finite in extent, width b, but in y and z direction it is infinitely large. And let us say that if we plot the mass fraction of a at this face of the slab, we have maintained it at a value w_{a1} and at the other face of the slab we maintain it as w_{a2} , so if the mass fraction is large here and the mass fraction is small here, the component a will diffuse through the slab from left to right and there will be a concentration gradient setup from the left to the right. So, this is the gradient of concentration of A which leads to diffusion of A. We will say we have gas A on this side, we also have the same gas on this side and a second component B is the slab; so gas A diffuses through the slab which is component B. In this particular case, one component is a gas, the other component could be a solid, it could even be a liquid layer.

Now, we have to consider a steady state and a one dimensional situation. Since the slab is stationary, it doesn't move and in steady state, if you take any plane here or here - a plane parallel to the, parallel to any face of the slab and in the slab - you will find that the flow of this diffusing component will be a constant through here, through here, through here because it is a steady state and the amount of gas crossing this plane should be the amount of gas crossing this plane should be the amount of gas crossing this plane should be the amount of gas crossing this plane. And that means we will have m dot a to be a constant independent of a and that means the mass flux of A would also be constant and uniform along the thickness of the slab.

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Diffusion through a slab (Contd) Since we have a steady-state, and a one-dimensional situation, using Fick's law, we get, $=$ constant $=-\rho D_{ab}\frac{dw_a}{dx}$ Assuming the density ρ of the medium to be a constant, we get = constant = $-D_{ab}\frac{d\rho_a}{dx}$

So again, since we have steady state and a one dimensional situation, the mass flux would be a constant that is independent of x, the location along the thickness of the slab, and by Fick's law this should equal minus rho into D_{ab} into dw_a by dx. Notice that since we have a steady state situation and a one dimensional situation, we use an ordinary derivative here and not a partial derivative. Now if we assume the density of the medium to be a constant - this would be a very good assumption if the thickness, if the density of slab b is much higher than the density of the gas a which diffuses through - generally it is a very good assumption. If the density of the medium is assumed constant, then the right hand side can be written in terms of the mass density of component a.

Now, here we have the derivate of rho a instead of the derivative of w_a . Now, this is the constant hence this also is a constant and now if the diffusion coefficient is a constant and - we have said that the slab is isothermal - since the slab is isothermal, it is expected that in the steady state the temperature of the gas will not change as it diffuses through the slab. And hence its diffusion coefficient is likely to be at some constant value; then we can straight away integrate the equation.

Diffusion through a slab (Contd) Since the diffusion coefficient is a constant, integration gives: $= D_{ab} \frac{\rho_{a1} - \rho_{a2}}{b} = \rho D_{ab} \frac{w_{a1} - w_{a2}}{b}$ and $\frac{w_{a1}-w_a}{w_{a1}-w_{a2}}$ which is a linear profile, similar to the steady-state conduction profile.

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If we integrate it from x equal to 0 to x equal to b along the full length of the slab, we will get the mass flux equal to the diffusion coefficient into the difference in the mass density of component a on two sides of the slab divided by the thickness of the slab. Or in terms of mass fraction, we have the mass fraction difference divided by the thickness of the slab multiplied by the diffusion coefficient multiplied by the density. Compare this with the result for steady state conduction through a plane parallel slab. You will find that the heat flux is represented or is equal to k into T_1 minus T_2 divided by b; I will write that equation again.

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The mass flux across a parallel slab, infinite parallel slab, in steady state and the corresponding equation for heat flux across a plane parallel slab in steady state is going to k T₁ minus T₂ divided by b. Notice the analogy and similarity. We have the mass flux, we have the heat flux; in heat flux there are no components, mass flux of component a. We have the conductivity of the material in mass transfer; we have the diffusion coefficient, thickness of the slab in the denominator. A geometric parameter doesn't change the same in case of conduction and mass transfer and now temperature is the analogous variable to mass density. We will keep noticing the analogies between conduction and mass transfer convection and mass transfer as we proceed.

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Diffusion through a slab (Contd) Since the diffusion coefficient is a constant, integration gives: $= D_{ab} \frac{\rho_{a1} - \rho_{a2}}{b} = \rho D_{ab} \frac{w_{a1} - w_{a2}}{b}$ and $\frac{w_{a1}-w_a}{w_{a1}-w_{a2}} =$ which is a linear profile, similar to the steady-state conduction profile.

If we integrate the equation not fully over the slab but from x equal to 0 to some x within the slab, then that integration and the previous integration will give us an expression for the concentration profile or mass fraction profile in the slab. And since we have assumed density uniform, this would also become rho a_1 minus rho a divided by rho a_1 minus rho a_2 equals x by b - again a similar result to the steady state conduction result. The density, mass densities, will be replaced by temperatures x, will be replaced x and b, will be just x and b; a linear temperature profile there, a linear concentration profile here.

In fact, if you solve the one dimensional steady state mass diffusion problem through a hollow cylinder, we will get an expression very similar to that for conduction across hollow cylinder steady state conduction.

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Here we have a cylindrical shell or a hollow cylinder inner radius r_i , outer radius r_o , inner concentration mass fraction wai, outer mass fraction wao. And you will notice that the diffusion mass flow of component a over a length L of the cylinder and the mass fraction profile of component a - the expressions are perfectly analogous to those for one dimensional steady state heat conduction through a hollow cylinder. And what is true for a case of a hollow cylinder is also true in the case of a hollow spherical shell; here too it is assumed that we have a spherical shell - inner radius r_i , outer radius ro, inner concentration or inner mass fraction w_i , outer mass fraction w_o .

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Diffusion through a hollow spherical shell $4\pi\rho L D_{ab}(w_{ai}-w_{ao})$ \dot{m}_a r_{o} $-w_{ai}$
- w_{ai} $rac{r}{1}$ $rac{r_o}{1}$ w_a $w_{a\sigma}$

Again, notice that the 2 expressions are perfectly analogous to the heat conduction equations. All that you would need to do is replace mass flow rate by heat flow rate diffusion coefficient, by conductivity, and mass fractions by temperature. Let us look at a simple problem; let us solve this problem

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We have to determine the rate at which hydrogen will diffuse through a steel plate 4 centimeters thick, face area of 2 meter square, uniform temperature of 400 K. Hydrogen diffuses through steel and causes embrittlement - that is a known factor. The concentration is given on the 2 sides as .1 and .01 kilogram per meter cube - this is mass densities.

Let us consider this problem; we have hydrogen diffusing through a 4 centimeter thick steel plate. Face area of the plate is 2 meter square and it is at a uniform temperature of 400 K. Concentration of hydrogen that is its mass densities on either side is .1 kg per meter cube and .01 kg per meter cube. The diffusion coefficient of hydrogen in steel at 400 Kelvin is given - 1.6 into 10 raise to minus 11 meter square per second. Notice how small it is but even then it is known that hydrogen diffuses slowly but surely through steel and causes embrittlement leading to pitting. Let us solve this problem; let us sketch the situation.

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We have a steel slab, the thickness b is 4 centimeters, $.04$ meters. D_{ab} is given as 1.6 into 10 raise to minus 11 meter square per second; uniform because it is given that the temperature is 400 Kelvin which also is uniform. The surface area of the slab A is 2 square meters; w_{a1} and w_{a2} are given - .1 and .01 kg per meter cube. Since these are kg per meter cube, this is actually rho a_1 and this is rho a_2 , steady state one dimensional situation.

So, our equation for diffusion rate of component a - hydrogen in this case - becomes, in terms of mass density of component A, area diffusion coefficient into the difference in mass densities divided by thickness of the slab. Substituting here - area is 2 meter square multiplied by diffusion coefficient which is 1.6 into 10 raise to minus 11 meter square per second multiplied by density difference which is .10 minus 0.01 divided by the thickness which is 4 centimeter so .04 units for density difference kg per meter cube and for the thickness of the slab meter. So, you will find that we have meter raise to 4 in the numerator, meter raise to 4 in the denominator. So, the units which remain are kilograms per second which are the proper units for the mass flow rate. Multiplying this out we will get this to be 7.2 into 10 raise to minus 11 kilogram per second, that is the answer we were looking for.

Now, notice that the diffusion coefficient is a significant function of temperature. If the temperature increases from say 400 to say 1200 Kelvin – 3 times - the diffusion coefficient will go up not just 3 times but not even by the square of 3 times, 9 times; it will be may be, it will go up by a factor of 5 or 6 and that means even the diffusion rate or if you want to call the leakage rate of hydrogen through the slab will also increase. This indicates that at higher temperature the chances of hydrogen embrittlement are large. This is enough for this lecture; we will continue in the next lecture.