Transport Phenomena. Professor Sunando Dasgupta. Department of Chemical Engineering. indian institute of Technology, Kharagpur. Lecture-43. Mass Transfer.

So far we have discussed momentum transfer and heat transfer and we have also worked what would be the type of transport, how can we press mathematically the transport inside a boundary layer, a hydrodynamic boundary layer and inside it a thermal boundary layer. For the case of hydrodynamic boundary layer we have seen how to obtain an analytical solution by converting a PDE which was originated out of the simplification of Naviar Stokes equation for flow inside a boundary layer on a flat plate.

So we used the method of combination of variables to obtain not only the velocity VX and VY inside the boundary layer, but also the gradient of velocity or at Y equals 0, that means that liquid solid interface, which was then used to obtain an expression for the friction coefficient CF. We then proceeded for solution of the or treatment of the turbulent boundary layers. And in turbulent boundary layers we saw that the situation became so complicated that it is not possible even to write the governing equation, the statistically it is having an universal velocity profile which would be valid in all regions of turbulent flow for flow over, even for a flow over a flat plate is extremely difficult.

So we have seen dividing the flow regime into 3 layers like viscous sublayer, the transition region and a turbulent core for the case of pipe flow. For each of these regions, there was a velocity profile. And there was also an entirely empirical velocity profile known as the one $7th$ power law which can be used to fit the experimental data, especially for those points situated near the centre. However this expression, even though it fits the data wells, it fails on the solid wall because you cannot evaluate the gradient of the velocity at Y equals 0, that means on the flat plate using one $7th$ power law, that was a major limitation.

So then we proceeded to obtain a momentum integral approach, an integral approach which resulted in a momentum integral equation and there with some approximation with an assumed value, assumed expression of velocity profile where the constants were evaluated with the boundary conditions that we have on the plate, namely no slip condition and at the edge of the boundary layer, that means where the velocity in the X direction would be equal to the free stream velocity and the velocity profile approaches the free stream with 0 slope. Using these conditions and assumed velocity profile, we could move ahead to obtain the,

what would be the boundary layer growth in the case of turbulent flow and what would be the friction factor expression.

We then used the same concepts for the treatment of the thermal boundary layer. In thermal boundary layer before that it is the equation of energy applicable inside the thermal boundary layer after the standard simplifications which are boundary layer approximations, this equation is coupled to the velocity boundary layer equation, namely the Naviar Stokes equation for flow inside the boundary layer. The coupling appears because of the appearance of velocity VX and VY in the energy equation. So it is a one-way coupling.

We showed in previous classes how to solve this thermal boundary layer growth and the velocity, when the temperature gradient at the solid liquid interface through the simultaneous solution of the momentum equation as well as the energy equation. So for laminar flow we have obtained an expression for Nusselt number which is the convective heat transfer coefficient multiplied by length scale divided by the thermal conductivity of the fluid, this Nusselt number was related to 2 dimensionless groups which appeared automatically through the nondimensionalization of the governing equation, namely Reynolds number and the Prandlt number.

So we got compact expressions of Nusselt number, the, with the Engineering parameter convective heat transfer coefficient embedded into the Nusselt number. So that is, the H is the one that we would like to evaluate and the corresponding dimensionless group is Nusselt number. So we got relationship between Nusselt number, Prandlt number and Reynolds number with a constant in front of it. But that was for laminar flow, I did not say anything about the turbulent flow inside a thermal boundary layer.

The treatment of turbulent flow inside a thermal boundary layer is more complicated, more complex because you are going to have transfer of heat not only by conducting an convection, there will be the formation of eddies and these eddies. And these eddies would carry additional heat, additional energy for flow when for the case when the flow inside the boundary layer turns to be turbulent. So the presence of eddies creates or imposes additional problems in solving the energy equation. $1st$ of all we do not know what would be the right form of energy equation.

So even if we express the energy equation in the same way as we have done for the case of momentum boundary layer, that is in terms of fluctuating components, it is almost intractable.

So we have to think of some ways to use the solutions that we have already obtained for the case of momentum boundary layer, both in laminar flow as well as in turbulent flow is there any way to use, to project those relations and or correlations for the case of turbulent flow in thermal boundary layer. So that means I am trying to find an analogy, a logical set of conditions which must be met, so that the results of momentum transfer in turbulent flow can be projected and to obtain the results connecting the dimensionless groups, relevant dimensionless groups for the case of turbulent flow inside a thermal boundary layer.

And if we can establish this transformation, then the same logic can also be obtained, can also be used to obtain the relation between the relevant parameters in for mass transfer inside the concentration boundary layer. The way we have the velocity boundary layer we have seen what is the thermal boundary layer. Similar to thermal boundary layer, I will also have the concentration boundary layer in which the species concentration would change from some value on the solid plate to a constant value in the free stream of the flowing solution above the solid plate.

So the results of, so it would be, it would be the objectives, as I mentioned at the beginning of the course the objective of this course would be how, why and when we can transform the relations obtained in hydrodynamic part of the boundary, solution of the hydrodynamic boundary layer, how can you use that as a solution of the thermal boundary layer and then for the concentration or the mass transfer boundary layer. So I am not going to do that right now, that would be the last topic of this course. So I would very quickly go through some of the salient features of the mass transfer process which is complicated because now we are dealing with mixtures of at least 2 components, maybe a solute and a solvent.

So at least 2 species are present in the case when we are having net transport of one species from the one point to the other. Now the net transport asks the species from one point to the other exactly like in the case of heat transfer, it can take place because of actual flow from point A to point B which carries component 1 from A to B. So that is due to the imposed flow of the solutions from point A to point B carrying component A from one location to the other, which is nothing but the convective motion of the species, the motion of the species due to convection imposed on the flow field.

There would be another way by which mass gets transported which is similar to the conduction heat transfer, heat transfer by conduction. So whenever there is a temperature gradient, even if there is no flow we will still have heat transfer because of molecular,

because of mobile means, because of molecular mechanism. So this conductive heat transfer which depends not only on the concentration difference but on the gradient of concentration between, gradient of temperature between 2 points, exactly similar phenomena exists for mass transfer as well which are aptly called the diffusive mass transfer.

So in diffusion or diffusive mass transfer, mass travel from one location to the other if there is an imposed concentration gradient, the concentration gradient may exist as a result of several conditions. But if there is a temperature, if there is a concentration gradient, then mass gets transferred from one point to the other. So similar to heat flux, similar to Fourier's law, similar to Newton's law of viscosity, the mass flux as in the case of heat flux is proportional to the concentration gradient. Think of this similarity with the temperature gradient.

So mass + is proportional to the concentration gradient and the proportionality constant with a - sign, since mass always travels from high concentration to low concentration, the concept of this expression is commonly known as the diffusivity of one in two. It is expressed in D, in the form D with a subscript AB which is the constant, which is the diffusion coefficient of A in B. Now some of the relations this is known as the fixed law of diffusion which like Newton's law or Fourier's law is a phenomenological equation, it cannot be derived, it can, it was arrived by looking at the data of many experiments over a large range of concentrations and it was found that a mass flux is always proportional to the concentration gradient.

So before we use fixed law and other physical boundary conditions in solving, in modelling the mass transfer process, the same way we have done for heat transfer, it would be, I would like to go quickly through the relations, the established relations in mass transfer that I am sure you already know, it is only going to be a recapitulation of what you have studied in your mass transfer 1 or mass transfer 2 courses. So our study of mass transfer and modelling of processes involving mass transfer, the mass transport process, we understand, we start with the fact, with the with the realisation that mass transfer is a more complicated process as compared to a momentum transfer all heat transfer because more than one species is involved.

So you will have at least 2 species and in multicomponent systems, we will have more than one species, more than 2 species which are present in the system and therefore the, not only the diffusion coefficients are going to be different, however the motion of the one species, the motion of the molecules of one species in a medium will start to affect the molecules of the

medium as well. So when component A is rapidly diffusing through a stagnant medium of , of B, then the motion of A molecules can create a movement, a flow of the B molecules as well.

So mass transfer is definitely more complicated than heat and momentum transfer, so we will quickly go through some of the modelling exercises of mass transfer, some of the relevant boundary conditions of mass transfer and then we will come back to last part of the course which is analogy between these different processes.

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O CET MASS TRANSFER DEFINITIONS MASS CONC. P. MASS OF SPECIES I PER UNIT VOL. OF SOL MOLAR CONC $C_i = \begin{bmatrix} i \\ m_i \end{bmatrix}$ No. of MOLES $n \times n \times ... \times n$ MASS FRACTION $W_1 = f_1 / f$ MOLE FRACTION $X_1 = C_1 / c$ $P = P_{A} + P_{B}$ mass DENSITY OF SOLN $P_{A} = C_{A} M_{A}$ $W = P_A/P$ $C = C_A + C_B$ MOLAR DENSITY OF SOLN $W_{A} + W_{B} = 1$ $x_{\lambda} + x_{\beta} = 1$ $\frac{\omega_{A}}{m_{A}} + \frac{\omega_{B}}{m_{B}} = \frac{1}{M}$ $X_A M_A + Z_B M_B = M$

So our study of mass transfer begins with some of the definitions that I am sure you, all of you are aware of or you have studied at some point of time, but I will go through it once again. So the mass concentration is essentially the mass of species I per unit volume of the solution, similarly the molar concentration is simply rho I by M i, by Mi is the molecular weight of component i. So this is the number of moles of I per unit volume of the solution. The mass fraction is simply divided as the mass concentration divided by the total concentration, the mole fraction XY is Ci by C, the molar concentration of one species divided by a focal molar concentration.

And of course if you add rho A and rho B for a binary mixture, then the mass concentration of A and mass concentration of B when added together would give you the mass density of the solution. And this rho A, as rho A is simply CA Times MA and W A which is the mass fraction is simply going to be rho A by rho. As with the case of mass density, so mass density, similarly the molar density of the solution is simply a sum of the individual molar densities

and we understand that XA which is a mole fraction, $XA + XB$ equal to 1, the same way weight fraction sum would be equal to 1 and these relations are self-explanatory.

So we have all seen these expressions before and we will see how these expressions will be used later on to understand, to express the mass transport process in a system where we have both convection as well as the diffusive mass transfer. So coming back to some of the other equations, other definitions that one can think of, one uses in mass transfer process.

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LOCAL <u>MASS</u> AV. VEL $\gamma = \frac{\sum_{i=1}^{n} P_i^T \vartheta_i}{\sum_{i=1}^{n} P_i}$ LOCAL MOLAR AV. VEL DIFFUSION VELOCITIES $v_{i} - v = D_{i} F F^{N}$ vec of i w.r.t. v $196 - 19^{*} = 1955^{4}$ vo. 2.

There is something called local mass average velocity which is simply rho I Vi divided by summation of rho I overall the species. So this is the mass average velocity, the same way you have the mass average velocity, you can also find out, will also express the molar average velocity where simply the mass concentration is replaced by the molar concentration. So the denominator is the total mass concentration whereas the denominator over here is the total molar concentration of the solution. Now whenever something, whenever a component moves in a, moves in the solution, then you can either fix the coordinate systems and keep them stationary.

So the 2 definitions of mass average velocity and molar average velocity that I have shown you before are with respect to stationary axes. Now the mass average velocity can also be used, let us say I have a portion of a solution in which there is a diffusing species A and this entire species has some mass average velocity with which it is let us say moving in this direction. However the species A present in it has a different velocity because it is also

diffusing as a result of the bulk flow as well as as a result of a concentration gradient imposed on it.

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LOCAL <u>MOLAR</u> AV. VEL $v^{\alpha} = \frac{\sum_{i=1}^{m} C_i v_i}{\sum_{i=1}^{m} C_i}$ DIFFUSION VELOCITIES $\sqrt{2}i - \sqrt{2} = \text{Diff}^{\text{H}}$ VEL. of i W.T. t. $\sqrt{2}$ $19i - 19^{*} = \text{Diff}^{4} \text{ VEL of } i$ $w.r.t. 20^{\circ}$ 120380

So if we want to separate the diffusion from the bulk motion of the fluid, then the diffusion velocity is something which is exclusively due to diffusion for a species A and therefore the diffusion velocity is expressed as Vi, that is the velocity of the ith species, subtract from that the local mass average velocity, so the difference in velocity, the additional velocity that the ith component has is over the mass average velocity is termed as the diffusion velocity. So Vi, the velocity of the Ith species - the local mass average velocity is termed as the diffusion velocity of I with respect to V.

Now the way you have expressed the diffusion velocity where the basis is taken as the local mass average velocity, you can take the basis as local molar average as in V Star. So the component velocity, the relative velocity of the component can be expressed with respect to the mass average velocity or with respect to the molar average velocity, both are diffusion velocities, one with respect to V, the other is with respect to the molar average velocity. So these are the 2 diffusion velocities that are commonly used for, in case of, in for mass transfer.

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 $\frac{\sqrt{3}}{2}$ = $\frac{\ln 1}{2}$ C i DIFFUSION VELOCITIES $\sqrt{2}i - \sqrt{2} = \text{Diff}^N$ VEL. of $i = \sqrt{2} \cdot \text{Tr} \cdot \text{Tr}$ $20^x = \frac{1}{2}(6x^2 + 6x^3 + 2x^2 + 2x^3 + 2x^2 + 3x^2 + 2x^3 + 2x^2 + 3x^2 + 3x^3 + 2x^2 + 3x^3 + 3x^2 + 3x^2 + 3x^2 + 3x^3 + 3x^2 + 3x^2 + 3x^2$

And this velocity, the velocity of this if you expand it, is simply going to be 1 by rho, 1 by rho times rho A VA + rho B VB in which if you take the ratio of rho A by rho, it is simply going to be the weight the weight fraction of component A and similarly V Star which is a local molar average velocity. If you expand this, it is simply going to be 1 by total concentration, then molar concentration of A, molar concentration of B and the velocities of A and B and CA by C is nothing but the fraction, the mole fraction of component A and mole fraction of component B. So these 2 relations directly follow from the definition of the mass average velocity or the molar average velocity.

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LLT. KGP MASS & MOLAR QUE FLUXES REL. TO STATIONARY COORDINATES ni = Pivi (mass) $Ni = CiVi (molar)$ REL. TO MASS AV. VEL V $j_i = p_i(v_i-v)$ (mass). $J_{i} = C_{i} (\varphi_{i} - \vartheta)$ (moles)

OL FLUXES REL. TO STATIONARY COORDINATE S n_i : P_i ϑ_i (mass) $Ni = CiU_{i} (molar)$ REL. TO MASS AV. VEL 19 $A: P_1(y, -y)$ (mass). $J_i = C_i (v_i - v)$ (mole). REL. TO MOLAR AV. VEL. 194 $P: (29, -19^*)$ $(mays)$ C_i $(\upsilon_i - \upsilon^*)$ (molar) CONC. GRADIENT -> FICK'S LAW (3)

Now since we have defined the diffusion velocities in this way, the diffusion velocities can then be converted to fluxes. So one would be a molar flux and the other would be mass +, so in terms of stationary coordinates, it is simply going to be rho I times V i, if you express it in terms of mass or if express in terms of moles, it is simply going to be C I Vi, these Vis are with respect to stationary coordinates. When you bring the same mass flux or molar flux and take the average velocity, average velocity V bar to be the basis, so relative to the mass average velocity, the mass flux or the molar flux denoted by j or capital J for the ith species is simply going to be rho i times the relative velocity square for the relative velocity we use the mass average velocity.

So it can either be expressed in terms of mass or it can be expressed in terms of moles. Same thing if we do in terms of molar average velocity, so this is in terms of stationary coordinates where the velocity is 0, where V is 0, so it is rho I Vi. If I have a mass average velocity and I express relative to the mass average velocity, it is simply going to be Vi - V. If I do it in terms of molar average velocity, it is going to be Vi - V Star for the case of mass and for the case of moles it is simply going to be Ci.

Now this flux, be it mass flux or molar flux is generally expressed, the molar flux where J star if you look at J star, this is the molar flux of the ith species when the flux is relative to the molar average velocity which is, so Ji times Ci times Vi - V Star, this molar flux is proportional to the concentration gradient. That is the statement of Fick's law. So Fick's law essentially tells us that the molar flux Ji Star is proportional to the concentration gradient. So Fick's law is simply the flux, molar flux of component A when expressed with respect to the average, molar average velocity is simply - DAB times divergence of XA.

So if C is constant, I can put C inside, it is simply the other way of writing it is time CA. So this for a rectangular coordinate system can be written as - DAB times Dell CA Dell X + Dell CA Dell Y + Dell CA Dell Z. So see the similarity that we have for the case, for decay with heat transfer and with mass transfer. So this is the statement of Fick's law and from our definition of molar flux, this is the definition of molar flux when expressed in terms of V start. So I expand it and CA VA is nothing but the smaller flux of A and then when you expressed this V Star, the formula would simply be CAVA $+$ CB VB by C. CA by C is the molar, the mole fraction, so your JA is equal to NA - XA times NA + NB.

Plug it in here and what you have is another form of, another form of Fick's law. So this is, this NA is relative to stationary coordinate and what it tells is that the molar flux of component A relative to stationary coordinates from here is a sum, is an algebraic sum of XA times $NA + NB$ where XA times $NA + NB$ is the flux due to the bulk motion of the fluid. So CA Times V star, V Star denotes the molar average velocity. So if we have a bulk velocity present, bulk motion present in the fluid, it is also going to contribute to a flux of A.

As I said the species A can move from point A to point B if there is a bulk motion. There may not be any difference in concentration, so a sugar solution, a constant concentration sugar solution may be forced, may be allowed to move from point A to point B by imposing a pressure gradient. There is no diffusion, since the concentration is same everywhere, but what you have a bulk motion of the sugar molecules from point A to point B. So this kind of bulk motion imposed by the flow only is the significance of the $1st$ that we have here which is XA times NA + NB.

So this is due to bulk motion. Sometimes in addition to bulk motion or even in the absence of bulk motion you have concentration difference. So if you have concentration difference or more correctly if you have a concentration gradient present in the system, then this is going to give rise to say diffusive motion of A, species A. So the total effective motion of species A is the algebraic sum of the species movement due to bulk motion and or the species movement due to the concentration gradient imposed due to certain conditions present in it. So therefore the problem of Fick's law is to be resolved, the $1st$ thing that needs to be resolved is what is, how to get rid of NB from the expression of NA. So NA is XA NA + NB - DAB Dell of concentration of A.

So $1st$ of all it may be mentioned that it is diffusion only process, that means there is no imposed bulk flow. So if it is a diffusion only process, then the $1st$ term on the right-hand side which signifies bulk motion can be dropped. So that is one way of getting rid of NB which is the unknown, which is which appears in this expression. So if it is a bulk motion, if it is a diffusive motion only situation, then this can be dropped. In some cases there would be a relation between NA and NB which arises due to some other factors.

For example it could be case of equimolar counter diffusion. That means for one mole of A moving in this direction, one mole of B is moving in the opposite direction. So if this is a case of equimolar counter diffusion where NA is going to be equal to - NB, for that specific case NA is going to be equal to - NB and therefore this term, the contribution of this term would be 0. So the expression would be same as that of diffusive motion only situation but for different reasons. Since it is equimolar counter diffusion, NA and NB would cancel out each other.

There are, in some cases the stoichiometry of the reaction if it is a reacting system, let us say 3 moles of A comes and reacts on a catalyst surface generating 2 moles of B which then travel in the reverse direction towards the bulk. So for every 3 molecules of A coming to a specific direction 2 molecules of B would have to travel in the opposite direction at steady-state in order to maintain the concentration at each point, either independent of time. So the concentration of A may vary, concentration of B may vary but the concentration at the fixed location is not, will not vary with time. So that is that is what the steady-state is.

So in some cases stoichiometry of the reaction, stoichiometry of the reaction taking place between 2 reacting components would give you some idea between the relation between what, how NA is related to NB. So in absence of any such generalisation, any such simplification, the expression to be used for the molar flux of component A will consist of 2 terms, one due to bulk motion and other due to the concentration gradient. So this DAB which is the diffusion coefficient of A and B for, they behave slightly differently for gases and for liquids, okay.

So most of them increase with an increase in concentration in temperature, so as the temperature increases, this DAB, it is a function of pressure, temperature and it is also a function of, it could be function of composition, composition of the gas mixture. So the gases, further gases and liquids, with increasing temperature DAB increases and at lowdensity it is almost composition independent for the case of or for the case of gases. So what we have then we need to see the similarity between DAB which is the mass diffusion

coefficient expressed either in terms of mass or in terms of mole, compare that with gamma which is mu by rho and compare that with K by rho CP which is Alpha.

So if you compare DAB, the diffusion coefficient of A and B, mu by rho, which is the kinematic viscosity and K by rho CP which is the thermal diffusivity, so momentum diffusivity, thermal diffusivity and mass diffusivity, all will have units of metre square for second. So these 3 are similar in nature, the mass diffusivity, the momentum diffusivity and the thermal diffusivity, they have the same unit as metre square per second and all of them denote the transport of mass, the transport of momentum or the transport of energy when you impose a concentration gradient, velocity gradient or a temperature gradient.

So this would be the beginning, the start of the, start of the analogy, finding the analogy between different processes heat transfer, mass transfer and momentum transfer. But before we reach that point what I would do in the subsequent process, 3 or 4, 4 or 5 classes after today is to show you examples by which $1st$ of all a shell component balance can be used, can be used to obtain the concentration profile of a specific component in a system where it is a diffusion only process, where both diffusion and diffusion and bulk motion convection is present and different ways by which NA can be related to NB.

The molar flux of A and the molar flux of B, what is the relation between them apart from counter diffusion, equimolar counter diffusion and so on. And finally the, like heat generation in the case of energy question, we can also have generation of a species due to reaction, generation or depletion of species due to reaction in a medium in which A is diffusing. So if A is diffusing and as it defuses, it reacts with another reactant B present in 8, then A is going to get depleted as it moves in the solution.

So reaction, chemical reaction, homogeneous chemical reaction can act as a source or a sink term in the mass balance equation. So when we write the shell balance of shell component balance, the same way we have done for, for the previous cases, heat transfer and momentum transfer. The source or sink term, for example in nuclear heat source or an electrical heat source, the equivalent of that in the case of mass transfer would be, if there is a reaction which is consuming A or a reaction which is producing A in the entire domain of transfer of A from point 1 to point 2.

So a homogeneous reaction would appear as a source or sink term in the governing equation. So contrary to that if it is a heterogenous reaction, that means if it is a, let us say it is a catalytic reactions well this is the catalyst surface and the reaction of A getting converted to B is going to take place only on the catalyst surface, it is a heterogeneous reaction. Therefore A diffuse and reach at this point when it gets converted to B and the products will diffuse back to the mainstream. In that case, since in the path of diffusing A, it does not encounter any reaction, generation or depletion.

The generation or depletion takes place only at a specified location, that is on the catalyst, heterogeneous reaction, this condition would appear as a boundary condition in the governing equation. So we have to keep in mind the difference between the heterogenous reaction and the homogeneous reaction, one in which it appears it appears as a source or sink term in the governing equation itself and the other variant appears as a boundary condition. So we will see examples of that, examples of modelling the process in the coming 4 or 5 classes and then we will finally move to the final part of this course which is to see, to evaluate the analogy between heat, mass and momentum transfer.