Transport Phenomena. Professor Sunando Dasgupta. Department of Chemical Engineering. Indian Institute of Technology, Kharagpur. Lecture-47. Mass transfer (Continued).

So we are going to work on another problem, this is going to be a tutorial class again, where we are going to look at the diffusion of one specific exhaust gas from an automobile where it reaches the catalyst surface of a catalytic converter through a one-dimensional diffusion only process. On the catalyst surface, the reaction takes place and the exhaust gas is converted to its higher oxides which is less harmful than the initial product which was coming out of the engine. So nitrous oxide is going to be converted to nitrogen oxide on the catalyst surface.

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So in words, the problem that we are going to look at is that we have nitric oxide emissions which are coming from an automobile, it can be reduced by catalytic converter and the reaction that takes place is NO + CO equals half N2 + CO2. The rate equation on the catalyst surface is given as - K1 triple, K1 double prime, it should be double prime, not triple prime. Since it is a heterogenous reaction, by our convention, the reaction rate constant has 2 primes on it showing that it is a heterogenous reaction taking place only on the surface of the catalyst. It can be assumed that NO reaches the catalyst surface by one-dimensional diffusion only process through a thin gas film of thickness L.

So if you can see this figure, we have a catalyst surface where, whose area is 200 cm² and the reaction rate constant of this reaction, that is K1 double prime CA, the reaction rate constant is 0.05 metre per second. And there is a thin film which is stagnant, whose thickness is 1 millimetre and Z is denoted from the catalyst surface, it is measured from the catalyst surface. So the flux, molar flux of nitrous oxide, nitric oxide tries to reach the catalyst surface by a one-dimensional diffusion process. The diffusion coefficient is provided as 10 to the power - 4 metre square per second and it has been measured that the concentration of NO at the exhaust gases, in exhaust gases is equal to 0.15.

The pressure of the exhaust gases and the temperatures are provided as 500 degrees centigrade and 1.2 bar, the diffusion coefficient, the mole fraction that is provided, you have to evaluate the 2, following 2 numbers. What is the mole fraction of NO at the catalyst surface? So the one that you have, the number that you have to calculate are the mole fraction of NO on the catalyst surface which is over here and what is the rate of NO Removal for a surface area of 200 centimetre square. So how much NO is going to be converted to N, to nitrogen when you have the reaction that is taking place over here and when the catalyst surface area is 200 centimetre square.

If you think of this problem, it is it is somewhat similar to a problem which we have done before, an exercise problem in which we have seen what would be the profile of concentration when we have instantaneous reaction taking place, that means are reactant that reaches the catalyst surface will immediately get converted into the product. But here we have a situation in which there is a finite reaction rate, so it would take some time for the reactant to get converted into the product and the rate of reaction is provided as its proportion, it is going to be proportional to the concentration of the reactant on the catalyst surface. Now if you think of the steady-state, then whatever be the amount of the reactant which is coming through the film to the catalyst surface must get converted by the reaction to the products. So in order to maintain steady-state, the rate of diffusion of the reactant towards the catalyst surface must be equal to the rate at which it gets converted into products. If that is not the case, then the concentration of the reactant or the product at a given point inside the film or on the catalyst surface will vary with time. So by our assumption of steady-state, we can now equate these 2 rates that is the rate of diffusion to rate of reaction on the catalyst surface. So it essentially gives us the 2 boundary conditions which would be required in order to solve the governing equations.

The 1st is known concentration at a given point where it has been given that the concentration of the reactant at the edge of the stagnant film is provided in terms of mole fraction and on the catalyst surface by our assumption of steady-state the 2 rates, the rate of diffusion must be equal to the rate of reaction. So our 1st objective for this problem would be to evaluate what is going to be the mole fraction of the reactant on the catalyst surface. So we would start this problem and once we are through with this problem, then we will shift towards deriving an expression, an equation, the species balance equation which we can use by choosing the proper coordinate system of the problem that we are interested to solve by choosing the appropriate equation and cancelling the terms one would be able to obtain the governing equation in a two-step process.

So we do not have to assume a shell across which we have to make the species balance. But that would be the next topic of today's class, initially in the 1st class we will start with the solution of the problem where automobile exhaust gases are converted to rather harmless products by a reaction, by reaction that is taking place on a catalytic surface. So we would start with this. Now if you see is this problem, you have done it before, what we need to do is, we need to assume a shell of some thickness Delta Z and we know that that the flux is coming in and some flux is going out, this is the flux of NO and no reaction is taking place in this shell, all the reaction that are taking place, they are on the catalyst surface.

So there would be no source or sink terms in here and it is a diffusion only process. So what you have then is, if I if I say this is N NO, this is the this is the flux in the flux multiplied by the area evaluated at Z - the same thing evaluated at Z + Delta Z would be equal to 0. So this would be the governing equation for solution of this problem.

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And when you divide both sides by Delta Z, your governing equation would look like d dZ, so this is problem on catalytic converter, so d dZ of N AZ where A is the reactant, would be 0, this is my governing equation and in this governing equation I have to substitute the expression for N AZ from 6 law, since it is, since it is a diffusion only process, the flux of A in the Z direction can be expect as - DAB d CA dZ.

So when you substitute that in here, what you are going to get is d2 C, D 2CA by DZ square is equal to 0 or C times D2 XA by DZ square is equal to 0, C being the total concentration which is a constant. So your governing equation would simply be D2 XA by DZ square equal to 0 where this is the mole fraction of component A which is this case is NO. So once you solve this you get a linear dissipation of XA in terms of Z and C1, C2, etc. are constants, constants of integration which are to be evaluated through the use of boundary conditions. So the 1st boundary condition is known concentration at a specific location at Z equals L, XA is equal to XA, XA times XAL.

And if you look at this figure, the value of XAL is provided and it is equal to 0.15. So I know that at one end of the film, stagnant film, the concentration of A is provided, so that is the 1st boundary condition. And of course the 2nd boundary condition would be the equality of diffusion rate and reaction rate on the catalyst surface. So when we use the 2nd boundary condition, what we are going to get is - DAB times C, C being the total concentration, D XA by DZ is equal to - K1 double prime denoting it is a surface reaction times C times XAS. So the reaction rate on the catalyst surface where the mole fraction of component A is equal to XAS and C being the total concentration, so this is equality of diffusion rate and reaction rate.

That is the relevant boundary condition at the catalyst surface. So what you would what you would get from here is the concentration will cancel from both sides and if you look at this expression, then D C, DX A DZ is simply going to be equal to C1, C2 being a constant, so what you have by plugging in the, plugging in this expression of XA, it would simply be equals DAB times C1 is equal to - K1 double prime XAS. So I have only used this expression of XA in here and obtained the expression for C1. So the 1st constant of integration can then be derived as K1 double prime by DAB times XAS. So this is the 1st constant of integration.

So therefore it would give you that X A to be equal to K1 double prime times DAB, XAS times Z + C2. So this is the 1st, this is the 1st condition that this is a simplified expression of this which we have obtained after evaluation of C1. But I still have to evaluate C2 which will follow from the 1st boundary condition which is at Z equals L, XA equal to XAL. So at Z equal to L, XA becomes XAL, this would give me the expression for C2.

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So since at Z equals L, XA equal to XAL, my XAL would be equal to K1 double prime XAS by DAB times L instead of X + C2. And you would get C2 to be equals XAL - K1 double prime XAS by DAB times L.

So the final form of the mole fraction distribution of component A in the thin film near the catalyst surface would be equal to K1 double prime XAS by DAB times Z - K1 double prime XAS by DAB times L + XAL. So we, we have written over here that the, this XAS is still unknown because we have said that at X equal to 0, XA is simply equal to XAS, this is, we have assumed it to be XAS, so an expression for XAS then can be obtained from here as to

the flow is, so if you if you take XA S common out of this and what you would get then is XA L divided by 1 + K1 double prime L by DAB. So I have obtained an expression for XAS, the mole fraction of component A on the catalyst surface in terms of the mole fraction of component A at the in the exhaust gases, the rate constant of the reaction, the diffusion coefficient of A in B, that is of A in B and the thickness of the film.

So once we have that, then I should be able to plug-in the numbers over here, so XAS would seem to be equal to XAL is 0.15 which has been provided in the problem, this is one + K1 double prime is 0.001 metre is that of L, so this is L times K1 double prime is 0.05 metre per second divided by DAB is given as 10 to the power - 4 metre square per second. So what you get then is the value of XA S and the value of XA S would be equal to 0.1. So this gives me the 1st part, part one of the problem, this is the concentration of the reactant in this case NO at the catalyst surface to be equal to 0.1.

So if you go back to the problem which we have, the picture of the problems, XAL is 0.15 and we have just now evaluated at XA S to be equal to 0.1. So therefore the diffusion from high concentration towards the low concentration would take place because of the difference in concentration in terms of mole fraction that exists between the film, the edge of the stagnant film and on the catalyst surface. And through this is the diffusion starts and when the reactants reach the catalyst surface, it gets converted to a product which then diffuses back to the mainstream. So at steady-state this must be equal to the rate at which it is taking place. So the 1st part of the problem has already been evaluated and now we should be able to find out what is going to be the expression and then the value of NAS.

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$$N_{AS}^{"} = -\frac{h_{1}^{"}C_{AS}}{1 + L h_{1}^{"}/D_{AB}} = 0.0187 \text{ kmol}$$

$$C = \frac{h}{RT} = \frac{1.2 \text{ ban}}{8.314 \times 10^{2} \text{ m}^{3} \text{ ban}} \times 773 \text{ k}$$

$$N_{AS}^{"} = -9.35 \times 10^{5} \frac{\text{ kmol}}{\text{ m}^{2} \text{ A}}$$

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$$N_{AS} = -1.87 \times 10^{5} \frac{\text{ kmol}}{\text{ A}} \times 0.02 \text{ m}^{2}$$

So starting with the expression which we have already obtained, this NA double prime that is the flux S, that is the flux, molar flux of A towards S would simply be equal to at steady-state the rate of reaction. And this is equal to - K times C times XAS. So the rate of diffusion is equal to the rate of reaction, so you get this formula and when you substitute the expression of XA S that we had just obtained in here, in this expression, what you would get as NA double prime S equals - K1 double prime times C times XAL divided by 1 + L K double prime by DAB. This part we have already evaluated, so only thing which is remaining is the unknown C. So let us see if we assume to be an ideal gas can be the total concentration, can be written in the form of an ideal gas using the ideal gas.

So P is given as 1.2 bar and the corresponding value of R is 8.314 integral to the power - 2, this is in metre cube bar kilo mole. So the value of the universal gas constant in the appropriate unit is this and the temperature is provided, temperature is provided at 500 degree centigrade, so at 500 degrees centigrade means it is going to be 773 Kelvin. So when you evaluate that, this C is going to be equal to, this C is going to be equal to 0.0187 kilo mole per metre cube. Now you can plug this value of C in here, this part is already known, so NA double prime S, you should be able to find out, - 9.35 into 10 to the power - 5 kilo mole per metre square times second.

You know the negative, the negative sign that appears in the value of NA double prime S and if you look at the picture once again, the flux of NO nitric oxide is essentially in the direction of - Z. So that is why the expression, the expression, the value of the, when I write the mass flux, the molar flux of A, that is going to have a negative sign in front of it. So the molar rate

of NO Removal for the entire surface, entire catalyst surface which is of the, which is of 200 centimetre square, I think this A is provided as 200 centimetre square, so the total amount which we denote as NAS would be equals N A double prime the flux multiplied by the area which would be - 9.35 into 10 to the power - 5, this is kilo moles per metre square times second into 0.02 metre square.

So your NAS, the flux of NO which is also equal to the rate of conversion of NO to NO2 would turn out to be 1.87 into 10 to the power - 6 kilos mole per second. So this is the 2nd part of the problem, so this part 2 of the problem which we have, which we have written. So in terms, so in terms of kilo mole per second, this gives you the total amount of A which gets converted into the products and through this methodology, this simple use of the governing equation, the boundary condition with the understanding that the rate of NO which is coming towards the surface must be equal to the rate at which it gets converted into other products and a known concentration at the edge of the film, we will, we were able to obtain what is the what is the distribution of a terms of mole fraction, distribution of the reactant in the thin film and equating the rate, equating the 2 rates, the diffusion rate and the reaction rate we have also obtained the rate of removal of NO for the catalyst area provided to us.

So this is another example of the use of shell balance, the boundary conditions and simple realisation of the fact that what steady-state means when it is a case of one-dimensional diffusion only process. So I hope that the problem is straightforward and you do not have any questions but if you do, please write to us and if there is any confusion, I will try to clarify it. So the next what we are going to do is imagining a shell in making the balance is easy as we have seen before, be it momentum balance, energy balance or in this case species balance, it would be easy the geometry is pretty straightforward and if you have a situation in which there is only, let us the concentration, the temperature or the velocity is a function only of X, let us say only of 1 direction, it is not a transient case.

But if it is a case of transient heat, mass or momentum transfer, where the heat, mass or the, where the temperature, the concentration or the velocity can be a function of both X and Y, 2 directions, 2 dimensions, then to imagine an area, to imagine a shell and taking care of all the in and out terms through convection, conduction, any source term, the presence of any time-dependent effects, they are complicated. So as before we will very quickly derive what is the species balance equation for such cases and then what will be the form of them in different coordinate system. So your job then reduces to only identifying what, which equation that

you have to use, which coordinate system you have to use, right it, cancel the terms which are not relevant and then get to your governing equation in a two-step process.

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But the 1st step for that is to know how we are going to solve, how we are going to derive equation, the component balance equation where diffusion, diffusion and time-dependent effects, transient effects of, all are present. So we are going to solve for the generalised species balance equation. So what we are doing is then the equation of change for multicomponent systems. And for that I am not going to draw everything here because we have done it extensively for other cases, so we are again taking the help of sum of a surface which has Dell Y, Dell Z and Dell X and we are going to use the conservation of mass of species A which is flowing into this.

So we have to take care of both conduction, which is essentially diffusion and convection which is with the flow. So mass can enter, the species A can enter this control volume either by diffusion, by diffusion as well as by convection. So the 1^{st} thing that we are going to write is in - out, that the rate of A, species A, time rate of species A coming into the volume by a convection and conduction process out + any generation or depletion, this generation or depletion due to the reaction which is taking place inside the control volume must be equal to the rate of change of A, the species A in the control volume.

So we are going to do this, so 1st start with, let us call it as 1, this is 2 which is in by convection, this is 3 which is in by conduction and this is 4 which is the rate at which A gets converted into other products. And for this I have 2 prime which would be the rate of convective transport of A out of the control volume and there will be 3 prime which is going to be the rate of conduction of A out of the control volume. So the 1st one is the time rate of change of A contained within the control volume, the 2nd one is the rate at which A enters the species A enters the control volume by convection and this is the rate at which A enters the control volume by conduction, 2 prime and 3 prime are simply the corresponding out terms for 2 and 3 respectively.

So we start 1st with 1 which is the rate of change of A inside the mass of A inside the volume element. So this would simply be equals Dell rho A by Dell T times Dell X Dell Y Dell Z. So this is the mass concentration of species A inside the control volume, so it is the time rate of change of mass concentration of A inside the control volume and when I multiply it with the volume, volume of the element, Dell X Dell Y Dell Z, what I would get is simply the term 1 which is the time rate of change of mass A inside the volume element.

And when I write, let us write 3, let us write 2 + 3 together, that means the rate at which species is being added to the control volume, I am not differentiating between convection and conduction right at this moment, so this is the rate at which A enters the volume element, species A enters the volume element and we realise that it is going to have a contribution of convection and conduction. So 2 + 3 would basically give you the flux of A, the mass flux, the mass flux of A in the X direction which is evaluated at X times Dell Y Dell Z.

Now we realise that the species A can enter through the X face, leave at the face at X + Delta X. It is going to enter through the Y face, leave at Y + Delta Y, it is going to enter through the Z face and leave at Z + Delta Z. So there would total be as we have seen before total 6 terms which would represent the net inflow of A inside the control volume. We are not

distinguishing between convection and conductive mode of species transferred at this moment. The NA, the mass flux of A that we are writing, we understand that it will have these 2 components embedded into it and we will at some point have to put in the right expression of NA that will consist of both conductive masses foreign convective mass transfer in and out.

So what I have done for the 1st term, that is A is this, and 2 + 3 which is going out, so this is the in term and is in term which is at X and this is the out terms at X + Delta X would be is little NA X multiplied, NAX evaluated at X + Delta X times Delta Y Delta Z. Similarly I will have 2 + 3 in through the Y face and 2 + 3 out through Y + Delta Y face, same for Z face and Z + Delta Z face. So these terms, there will be total 6 terms, 3 for in and 3 for out, I am not writing all of them. The the derivation of this is provided in Bird, Stuart, Lightfoot, so you can see the Bird, Stuart, Lightfoot for complete derivation but fundamentally the rate of change of A in the volume element is this and these represents the in and out of X face.

Similarly I should have in and out at Y face, in and out at Z + Delta Z face. And let see the sum A, the rate of production of A and we understand this is going to be by chemical reaction, if it is by chemical, it has to be by chemical reaction, then this is going to be R A multiplied by Dell X Dell Y Dell Z, so this is the mass of A generated or consumed by reaction multiplied by the volume element. So now I have identified all terms, the time-dependent term, which is this, the generation or reaction terms which is this and all these are in and out which are these terms.

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So the when I express the algebraic sum of this, put all these terms in here, divide both sides by Dell X Dell Y Dell Z and taking the limit when Dell X Dell Y Dell Z, all tend to 0 as we have done previously so many times, the final expression, the species balance equation, the mass balance equation would simply turn to be Dell rho A, species concentration, species concentration of A expressed in terms of, in terms of mass times this is + Dell N A in the X direction by Dell X + Dell NA in the Y direction by Dell Y + Dell NA in the Z direction by Dell Z is equal to the rate of reaction of A.

So this equation then is the species balance equation, where this gives you the time rate of change of mass concentration of A inside the volume element, these 3 are the rate at which A is being, the net rate at which the species is being added to the control volume. But we understand, we understood that this NA will have 2 contributions, one contribution is going to be from the diffusive mass transfer, the 2nd contribution will have to be from day, from a convective mass transfer. We are not separating them out at this point but we will have to do that eventually in order to obtain the variation of concentration of A inappropriate terms considering all these different ways by which A can be added to the system.

And the last term on this would be the rate of reaction, that is the rate at which A is produced or A is consumed in the system. So in the next part of the, part of the class I am going to substitute the appropriate expressions for NAX, NAY and NAZ and then see how a compact expression for the variation of the species concentration inside, inside a volume at a point fixed in space can be obtained in terms of all these inflow terms, the reaction terms and the sum total of this result would be change in mass concentration of A with time at a fixed location in space. So this is the background, this equation is the background based on which we will develop slightly more advanced expression for the species balance equation.