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Lecture - 35 Quasi-Steady Analysis of Simultaneous HT, MT and Chemical Reaction

Welcome to the MOOCs course Transport Phenomena of Non-Newtonian Fluids. The title of today's lecture is Quasi-Steady Analysis of Simultaneous Heat Transfer, Mass Transfer and Chemical Reactions. So, in this lecture and then coming couple of lecture, we will be discussing a problems where simultaneous heat and mass transfer + in addition to that there may be reactions also such kind such situations, such problems we will be discussing.

But we will be taking pseudo steady state or quasi steady analysis. What does it mean by? Till now you know most of the problem whether it is associated with the momentum transfer or heat transfer or the ongoing mass transfer we have taken only steady state problems. Indeed, when we take the time dependent problems then solution may become very difficult and analytically doing or obtaining solution is very difficult.

We may need to move forward for the numerical solution and under such conditions. But however what we do? We take in between step up steady and then completely time dependent that is quasi steady or pseudo steady state problem we will be taking, where we will try to incorporate the time information as well right. So, today we will be taking a case where simultaneous heat transfer mass transfer and chemical reactions are occurring.

And then under such conditions if we wanted to apply the quasi-steady models in order to get the solution. So, how to do that is what we are going to see.

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For this purpose, we are taking a problem on combustion of carbon particle. We have a single carbon particle and then it is being combusted right and then it is producing carbon monoxide. So, one mole of carbon, half mole of oxygen reacting and then producing one mole of carbon monoxide that is what situation we are taking. So, combustion of carbon occurs primarily through the following reaction at carbon surface. There may be other reactions also may be taking place so but we are restricting ourselves to one reaction that is given here right.

Now, consider a spherical carbon particle species C of radius R suspended in a gas mixture under pseudo steady conditions. The carbon particle that we are considering we are taking spherical particle. In reality, it may not be necessary that you know carbon particle where the combustion going on may be spherical it is not necessary, but for simplicity we are taking spherical particle. The particle radius is R; obviously, this is changing with respect to time because as time progresses the reaction progresses and then combustion of the particle takes place.

And then; obviously, it size gradually decreases. So, this is function of time right and then we are designating this species carbon as C, oxygen we will be taking A and then carbon monoxide as B ok and this situation we are taking under pseudo steady conditions. Assume that gas contains only oxygen and carbon monoxide. Oxygen let us designate as a species A, carbon monoxide as species B ok. Then mole fractions $x_{i\infty}$ and temperature T_{∞} far away from particle are known. ∞ stands for infinite distance, far away; infinite in the sense it will not be infinite may be compared to the radius of the particle the far away conditions may be 100 times R or 200 times R that is what in general taken as a kind of faraway distance ok.

And then $x_{i\infty}$ in the sense $x_{A\infty}$, $x_{B\infty}$, $x_{C\infty}$ that is A B C composition for at far away distance are known, i stands for you know A, B or C it can be anything. Reaction is very fast; that means, moment the oxygen is coming and then reaching the carbon particle immediately it is reacting and then forming carbon monoxide that is what it mean by fast reaction.

Now, one of the previous lectures also we have taken how to do the mass transfer analysis or how to consider the fast reaction contribution in the overall mass flux those problems we have taken both for heterogeneous and then homogeneous situations. So, there also we realize that if the fast reaction is very fast. So, what happens? The concentration of the reacting species immediately falls 0.

That means, x_A at r = R = 0, because this A is oxygen and then moment it reaches the carbon surface immediately it reacts and then forms carbon monoxide which is species B right. And then particle is small enough that Peclet number is very very smaller than 1 for both heat and mass transfer. So, what does it mean by if it is very very small? So, two things you know we can understand from this one.

So, whatever the transport is there that is occurring because of the molecular mechanism only right, conduction or you know diffusion depending on the transport heat transfer or mass transfer + we another thing we can understand this symmetry is there. So, that whatever the concentration profile is there and temperature profile is there they are function of r only they are not function of θ and ϕ coordinates.

This is what we can conclude from this assumption from this assumption. And then if the Peclet number is very very smaller than 1 then; obviously, these two are physically also more reliable. So, our problem has simplified. So, rather finding x as you know function of all three coordinates r, θ , ϕ . Similarly, temperature finding as function of all coordinates r, θ , ϕ it has simplified by this assumption that you know the concentration and temperature are function of r only because of the symmetry and then molecular mechanism is leading the transport process.

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So, that is the problem statement. So, first part of the question is that relate fluxes at the surface and then relate reaction rate to $\frac{dR}{dt}$. So, this R as function of time this is what we know. So, rather directly relating the flux N to R or you know relate the reaction rate let us say R_s if reaction rate is R_s then relating it to R as function of a time, what we are what we have been asked? We have been asked to relate this fluxes to $\frac{dR}{dt}$ and then this reaction rates also to $\frac{dR}{dt}$. That is what we have to do right.

We do not want to relate to directly R function of time, but we wanted to we have been asked to relate this flux and then reaction rate to $\frac{dR}{dt}$.

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So, what is the next part of the problem? Determine O_2 flux at the surface that is N_{A0} . Why at O_2 ? Because the carbon particle is stationary right, the bulk is having O_2 and CO in general right. Because both of them are present you know at any time t, let us say at any time t I am not saying that initially at some time where the reaction has already progressed because we have to relate all these quantities to time t ok.

So, when this O_2 comes to the surface then only reaction takes place and then that reaction is very fast. So, at what rate this O_2 is reaching or what is the flux of this O_2 at the surface that is N_A ok at r = R that we are calling N_{A0} . So, that N_{A0} which is nothing but N_A at r =R that we have to find out because it will tell at what rate the O_2 is reaching the carbon particle. So, then accordingly the combustion will also progress ok. Relate the heat flux and then reaction rate at the particle.

That is the other question, q and then r or q_0 and then this R_s let us say reaction rate is R_s . Then, this also we have to relate, we have to find out at the particle surface that is at r = Rwe have to find out them. Then, determine the particle temperature T_0 . What is T_0 ? T_0 is the temperature at r = R that is at the particle surface this we have to find out and then this is function of time actually, isn't it.

Why? Because you know as the reaction progresses the more combustion takes place and then temperature gradually changes ok. So, that also we have to find out ok.

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Now, schematically this is what we have; we have a carbon particle whose radius is R (t). And then, gases stream or this surrounding of the carbon particle is occupied by the gas which includes oxygen and carbon monoxide. Far away from particles $x_{i\infty}$ and then T_{∞} are known right. So, these are the things only known, nothing is known actually.

Then, just imagine you know even if it is a steady state problem if you know only far away conditions, you do not even know what are the conditions at the surface neither in terms of concentration, neither in terms of flux, and neither in terms of temperature do you not know any condition at the surface. So, then even steady state problem you cannot solve this. In fact, because of that constraint of not having any condition, any information about the concentration or temperature at the surface we have to or we are forced to go for some kind of a pseudo steady approach or quasi steady analysis right.

So now, what I do? I will have a line dotted line here just outside of a circle right. And then I am designating it as R^+ right which is nothing, but very first layer towards gas stream right. And then inside the circle or inside this carbon particle I am drawing another circle which is I am calling R^- which is the very first layer towards the particle; towards the particles side.

Basically, this $R^+ R^-$ are at the surface only they are not different location, but for mathematical simplicity we are you know representing one towards the particle and then another phase towards the gas side. Because we have to do so many interfacial balances

here so that this becomes very essential ok. So, that is the reason these two layers now this is what we are going to have, we should have this picture in mind throughout the class of all the slides today right.

So, this is one and then what happens they are actually they are at interface, but finally, you know after doing the balance we remove; we remove this $R^- R^+$. And then we have you know superscript or subscript o in indicating that is evaluated at the surface ok. This is the notations that we need to you know keep in mind until we complete the problem right.

Now, let A is O₂ and B is CO and then C is carbon this is given. Peclet number is very very smaller than 1 for both heat and mass transfer because of that one we can have a spherical symmetry so that x_i is function of both r and t only, but it is not function of θ and ϕ ok. Now, the first part of the question relate fluxes at the surface and relate reaction rate to $\frac{dR}{dt}$. So, we will be developing some relations.

Let us say N_{Ar} you know as you know N_{Ar} as function of $\frac{dR}{dt}$, then N_{Br} as function of $\frac{dR}{dt}$ or R_s as function of $\frac{dR}{dt}$ these kind of relations that we are going to develop. That we can do only when we do the balances right. So, in the interfacial species balance which follow a subscript "o". So, we are going to write let us say the flux N_{Ar} at r = R we will be calling it N_{A0}.

Similarly, N_{Br} at r = R we will be calling it N_{B0}, this 0 is following indicating that interfacial species balance coming out because of the interfacial species balance. And it denote gas quantities evaluated at the surface that is at $r = R^+$. Towards $r = R^+$ only gaseous species are there because carbon is not going into the gaseous state because it is a solid carbon is a solid particle right.

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• carbon: $\left(N_{C}' - C_{C}' \frac{dR}{dt}\right)\Big|_{R^{+}} - \left(N_{C}' - C_{C}' \frac{dR}{dt}\right)$ • At R^+ , carbon is non-volatile $\rightarrow N_c = 0$ and $C_c = 0$ • At R^- , stationary and pure carbon, so $N_C = 0$ $\frac{dR}{dt} = \frac{R_{SC}}{C_C} \to (1)$

Then for the carbon if you do the balance then what you have? Towards the gaseous side minus towards the particle side should be equals to the rate of reaction right. Towards the particle side or gaseous side it is same, $\left(N_C - C_C \frac{dR}{dt}\right)|_{R^+} - \left(N_C - C_C \frac{dR}{dt}\right)|_{R^-}$ they are not same, but similar mathematically similar, but quantity wise they are very different ok.

And this difference has to be balanced by the rate of reaction right. So, now, here R^+ is what? R^+ is the location towards the gas side; towards the gas side there is no carbon at all; it is only gaseous components are there carbon is present only towards the particle side. So, C_C is 0 and then; obviously, N_C would also be 0 right and then R^- , towards R^- , C_C is pure carbon.

It is a pure carbon towards the particle side it is pure carbon because whatever the gaseous product they are forming including CO and then reactant O_2 they are once the oxygen reaching the carbon particle surface, once the oxygen reaches the carbon surface you know then immediately the reaction takes place and then CO forms that CO also goes into the bulk of the reaction bulk of the you know let us say.

So, moment this O_2 comes here immediately CO will form and then this will go and then diffuse to the bulk gases stream right. So; that means, what happens at R^+ , there is no carbon only gases streams are there and these CO etcetera they are not coming into the carbon particle that is what it mean by, they are not coming inside the particle gases streams are not penetrating into the carbon particle. They are you know diffusing from the surface after reaction they are through the mechanism diffusion they are going back into the bulk stream, bulk gases stream right. Similarly, carbon particle is a stationary carbon particle whose size is decreasing because of the reaction, but carbon as a particle, as a solid it is not going into the gases stream right. So, these constraints we are going to apply for all three components carbon, oxygen and then carbon monoxide when we do the balance.

So, C_C is pure. So, then inside the particle there is no flux. So, then N_C is 0 and then R_{SC} is that you know rate of reaction with respect to carbon, C stands for carbon right. So, at R^+ carbon is non-volatile. So, N_C is 0 and then C_C is also 0 because towards gas there is no carbon at all. So; obviously, C_C would also be 0. At R^- stationary and pure carbon is there.

So, N_C is 0, C_C would be there. So, then what we get? $\frac{dR}{dt} = \frac{R_{SC}}{C_C}$, or $C_C \frac{dR}{dt} = \frac{R_{SC}}{C_C}$ rate of reaction of that component with respect to C; rate of reaction with respect to C divided by the concentration of a C that is carbon. So, this is one equation that $\frac{dR}{dt}$ we related to rate of reaction ok.

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Then, similarly if you do the oxygen balance A stands for oxygen. So, $\left(N_A - C_A \frac{dR}{dt}\right)|_{R^+}$ that is towards gases stream $-\left(N_A - C_A \frac{dR}{dt}\right)|_{R^-}$ that is towards the particle side should be

balanced by the R_{SA} that rate of reaction with respect to A. So, this R^+ is the location of towards the gas side; towards the gas side at surface this is at the interfacial interface right particle surface. At the interface N_A is there, the oxygen is reaching the surface and then only the reaction combustion reaction is taking place between carbon and then oxygen.

So, it should be there. So, at the surface we have already designated that you know quantities are provided with $0 N_A$, so, N_{A0} , N_B so, N_{B0} like that, but this C_A . What should be C_A ? The concentration of oxygen it is coming with certain concentration and then reaching the particle surface, but moment it reaches the particle surface immediately it is reacting and then carbon monoxide is forming.

We are assuming that the 100 percent oxygen is being consumed for the combustion with the carbon particle. So, then its concentration is 0 at the surface it is 0. And then R^- ; R^- is towards the particle size towards the particle size there is no gas diffusing into the gas is not penetrating inside particle gases are coming, oxygen is coming and reacting on the surface. And then carbon monoxide is forming that carbon monoxide is also diffusing back to the bulk gas stream, but it is not penetrating into the carbon particle.

So, both N_A and then C_A would be 0; that means, N_A = R_{SA}; that N_A at r = R we are calling N_{A0}. So, N_{A0} = R_{SA}. So, flux we relate it to the rate of reaction.

• CO: $\left(N_B^2 - C_B^2 \frac{dR}{dt}\right)\Big|_{R^+} - \left(N_B^2 - C_B^2 \frac{dR}{dt}\right)\Big|_{R^-}$ $= R_{SB}$ • At R^+ , $N_B = N_{B0}$ and $C_B = C_{B0}$ • At R⁻, only pure carbon inside particle region, · so concentration and flux of other components should be zero • $\Rightarrow N_{B0} - C_{B0} \frac{dR}{dt} = R_{SB} \rightarrow (3)$

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Now, similarly if you do for carbon monoxide, B stands for carbon monoxide. So, $\left(N_B - C_B \frac{dR}{dt}\right)|_{R^+}$ that is towards the gases stream $-\left(N_B - C_B \frac{dR}{dt}\right)|_{R^-}$ that is towards the particle side should be balanced by the rate of reaction with respect to the carbon monoxide B right. So, now, here at R^+ moment the oxygen is coming and then reacting with the carbon particle immediately on the surface you know carbon monoxide is forming that is diffusing back into the bulk gases stream.

So; obviously it would be there, flux of carbon monoxide would be there something we do not know we will find it. So, that we are calling N_{B0} because any quantity whether it is concentration or flux or whatever if it is at the interface we are designating, we are using subscript 0 ok. And then this C_B ; C_B is nothing, but the concentration of a carbon monoxide towards the gas side.

It is towards the gas side. So, that definitely when a carbon particle is reacting with a oxygen particle carbon monoxide is forming. So, definitely it is there, how much it is we may not be knowing, but it will be there. So, both these terms would be there here in this case of CO, but R^- case that is towards the particle says to the interior of the particle gases are not being diffused or penetrated.

So, their flux their concentration would be 0. So, what we have? $\left(N_{B0}-C_{B0}\frac{dR}{dt}\right) = R_{SB}$ fine. So, here the flux and then rate of reaction both are related to $\frac{dR}{dt}$, first case only rate of reaction was related to $\frac{dR}{dt}$ in the case of carbon particle. In the case of oxygen only flux and N_{A0} was related to the rate of reaction right. In the case of carbon monoxide both flux and then rate of reaction are related to $\frac{dR}{dt}$ right.

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•
$$C(s)+1/2 O_2(g) \rightarrow CO(g)$$

• Reaction stoichiometry: $R_S \equiv \frac{R_{Si}}{\xi_{i, c}}$
• where $\xi_A = -\frac{1}{2}$; $\xi_B = 1$; $\xi_C = -1$
• $R_S = -2R_{SA} = R_{SB} = -R_{SC} \rightarrow (4)$ $P_A = \frac{P_{AB}}{-\frac{1}{2}} = \frac{P_{AB}}{1} = \frac{P_{AB}}{-\frac{1}{2}} = \frac{P_{AB}}{$

Now, we look at the stoichiometry. So, 1 mole of solid carbon particle is reacting with half mole of an oxygen gas to produce 1 mole of a gaseous carbon monoxide right. Then reaction stoichiometry overall reaction rate if it is R it should be written like approximately $\frac{R_{Si}}{x_i}$, i stands for any component A B C here that is you know oxygen, carbon monoxide or carbon anything, x_i is nothing but stoichiometric coefficient here of the reaction.

So, with respect to A; A is for the oxygen it should be minus 1, with respect to B product B is carbon monoxide. So, it should be + 1 and with respect to carbon reactant. So, it should be - 1 from this reaction coordinate this one we are getting. So; that means, we can write $R_S = \frac{R_{SA}}{-1/2} = \frac{R_{SB}}{+1} = \frac{R_{SC}}{-1}$.

The +1; + – symbols we are using indicating if it is a product then +, it is a reactant then it should be – ok. So, that is $R_S = -2R_{SA} = R_{SB} = -R_{SC}$. So, this equation number 1, 2, 3, 4 these 4 equations we are going to use existentially in you know remaining part of the lecture. (Refer Slide Time: 24:50)



So, we should remember them or we should write them wherever we need them ok. So, next step is that combining interfacial balances and stoichiometric information. So, first balance that is in the case of carbon particle when we did what we got? We got $\frac{dR}{dt} = \frac{R_{SC}}{C_C}$ and then from this equation number 4, R_{SC} is nothing, but $-R_S$ right

That means, $\frac{dR}{dt} = -\frac{R_S}{C_C}$. So, now, this $\frac{dR}{dt}$ and flux we are relating to the rate of reaction you know with respect to the overall reaction R_S rather writing individually with respect to the A, B or C ok. Then second balance in the case of oxygen what we got? $N_{A0} = R_{SA}$ we got now, but equation number 4; according to equation number 4 from that is stoichiometric information that we had.

So, R_{SA} is nothing, but $-\frac{R_S}{2}$. So, $N_{A0} = -\frac{R_S}{2}$. Then third equation that is when we do the balance for carbon monoxide we get $N_{B0} - C_{B0}\frac{dR}{dt} = R_{SB}$ and this R_{SB} is nothing, but R_S from equation number 4. So, R_S and then this $-C_{B0}\frac{dR}{dt}$ I bring it to the right-hand side, so that I can have $+C_{B0}\frac{dR}{dt}$ right.

So, now $R_S + C_{B0} \frac{dR}{dt}$ is nothing, but $-\frac{R_S}{c_c}$ that is what we get just now. So, now, from these two terms R_S if I take common $1 - \frac{C_{B0}}{c_c}$. Now, at the surface; at the surface C_{B0}

concentration is going to be very much less compared to C_c because moment it forms after reaction between C and O₂ immediately diffuses back to the bulk of the stream.

But the carbon is there only whatever its concentration is there its size may be reducing particle size may be reducing with respect to time. But the concentration wise it is going to be there only whatever the initial concentration maximum is there pure carbon that would be there till the last drop of that carbon particle is reacting. So, compare to C_C , C_{B0} is going to be very small.

So, then this ratio is going to be you know close to 0. So, then $R_S \left(1 - \frac{c_{B0}}{c_C}\right)$ we can write R_S multiplied by 1 and then this R_S is nothing but from this equation we have R_S is nothing, but $-2N_{A0}$, that is $N_{B0} = -2N_{A0}$ that is what we had ok. So, finally, $\frac{dR}{dt} = -\frac{R_S}{c_C}$ and $N_{B0} = -2N_{A0}$.

So, in addition to first four equations, this 5th equation is also going to be very essential for our remaining lectures we do not need to remember any other equations they will be derived subsequently one after other because of the mathematical simplification. But, in coming all rest of the mathematical simplification one or other of this 1 to 5 equations would be used ok.

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B) O_2 flux at the surface, i.e., N_{A0} : \$ MODIVER • Species conservation in gas (In Spherical Coordinates): $(\nabla \cdot N_i) + R_{Si} \Rightarrow \frac{\partial}{\partial r} (r^2 N_{ir}) = 0 \Rightarrow (r^2 N_{ir}) = f(t)$ only $r = -2N_{Ar}$ for all r (using surface fluxes relations) we know that $N_{Ar} = -cD_{AB}\frac{dx_A}{dr} + x_A(N_{Ar} + N_{Br})$ $= -cD_{AB}\frac{dx_A}{dr} + x_A(N_{Ar} - 2N_{Ar})$ $\frac{-cD_{AB}}{(1+x_A)}\frac{dx_A}{dr} \to (6)$ NA

So, now the second part that is O_2 flux at the surface. That is N_{A0} actually N_{Ar} at r = R we are finding that we are calling N_{A0} . Because it is at the surface at the interfacial locations whatever the quantities are there they are replaced by you know they are represented by subscript o as well. So, species conservation in gas that is you know you have a particle and then surrounding gas also you are taking the spherical geometry like this.

So, then in spherical coordinates species conservation equation for you know gaseous region if you do which is in the spherical coordinates you have $\frac{\partial C_i}{\partial t} = (\nabla . N_i) + R_{Si}$ right. In the gas there is no reaction taking place, in the gases stream there is no reaction is taking place whatever the reaction is taking place that is taking place right at the carbon particle surface and then product carbon monoxide is diffusing back to the bulk stream of a gas right.

So, this is 0 and then also we take this $\frac{\partial c_i}{\partial t}$ also 0 for the time being, we are going to consider that way anyway. So, then what we get this is having N_i; N_i would be having N_i, N

So, that when you expand this one in spherical coordinates after removing the $\frac{\partial N_i}{\partial \theta}$ terms or $\frac{\partial N_i}{\partial \phi}$ terms this is the only term we are going to have ok. This is coming by expansion of this one and then striking of N_i, N_i terms after simplification this is what we are having that is equals to 0. Now, r² N_{ir} is equal to some constant with respect to r, but that constant is function of time. That is what taken that is what we are taking right.

So, this constant whatever is there that is constant with respect to r because with respect to r we are integrating, but it is function of time only. So, that is what we are bringing in that is how we are bringing in the effect of time here in the quasi steady analysis. What is this f (t) and in all that we are going to find out in the subsequent steps right.

Further, we understood just previous slide equation number 5, $N_{B0} = -2N_{A0}$ so; obviously, N_{Br} should be $= -2N_{Ar}$ for all r that is for all r. We have done at the interface, but that is going to be true for all r values because of this Peclet number very very small right. So, N_{Br} should also be written as $-2N_{Ar}$ in compare to which is consistent with the $N_{B0} = -2N_{A0}$ ok.

So, we know that combine flux $N_{Ar} = -cD_{AB}\frac{dx_A}{dr} + x_A(N_{Ar} + N_{Br})$ in place of N_{Br} we write $-2N_{Ar}$, then what we do we write N_{Ar} terms one side and then remaining terms other side. So, then we have $N_{Ar} = -\frac{cD_{AB}}{1+x_A}\frac{dx_A}{dr}$. Now, we want this N_{Ar} at r = R, that is N_{A0} we want that we can do only when we know what is this you know right side function of x_A .

Because here also we do not know what is x_A and then how it is changing with r. So, if we stop here it is an incomplete equation, it is not usable right. So, what is this x_A as function of r that also we have to find.

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Now, we simplify equation number 6 for x_A . So, equation number 6 is this one in the previous slide that we have derived. So, $\frac{dx_A}{dr}$ we are writing one side other terms we are writing other side. So, now, if you wanted to find out this x_A as function of r, what is this N_{Ar} as function of r that we should know. Indeed, that we already know that $r^2 N_{Ar}$ is function of time, but what is this function of time we do not know maybe there may be r^2 terms r terms may be there. So, we cannot you know directly write this one as f (t) and then integrate it right.

For that what we try to do? We try to get over any of such kind of things are there. So, then we try to get over of them. How we can do? We just now had $r^2 N_{Ar} = f(t)$ right. So, this one if you write $r^2 N_{Ar}$ is equal to constant from this equation $\frac{d}{dr}(r^2 N_{Ar}) = 0$ which

we derived previous slide ok. So, now, this $(r^2 N_{Ar}) = C_1$, the C_1 and same in place of writing f (t) I am writing C_1 so that I can write $N_{Ar} = \frac{C_1}{r^2}$ right.

Now, at r = R, N_{Ar} is nothing, but N_{A0} that is the designation you know notation that we are following that should be $\frac{C_1}{R^2}$ right. That means, $C_1 = N_{A0}R^2$; that means, this C_1 if I use here in this equation I get $N_{Ar} = N_{A0}\frac{R^2}{r^2}$. So, work done. So, now, this N_{Ar} you can substitute here and then you can do the integration to get x_A as function of r right.

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So, in place of N_{Ar} we can write $N_{A0} \frac{R^2}{r^2}$ remaining terms are as it is. Then we take this $\frac{dx_A}{(1+x_A)}$ one side and other terms on other side so that by integrating left hand side we have $\ln(1 + x_A) \mid_{x_A=0}^{x_A=x_{A\infty}}, x_A = 0$; that means, at r = R.

As already mentioned at r = R when the oxygen comes and then reaches the particle surface immediately it reacts with the carbon and then reaction nature is very fast. So that, at any time t its concentration would be 0 because immediately it is reacting with the carbon and then carbon monoxide is forming. So, right at the surface its reaction at any time we can take it as a 0.

So, that is $x_A = 0$ at r = R and then $x_A = x_{A\infty}$ at $r = \infty$ right, $= -\frac{R^2 N_{A0}}{c D_{AB}}$ integration of $\frac{dr}{r^2}$ is $\left(-\frac{1}{r}\right)|_{r=R}^{r=\infty}$. So, it should be $+\frac{1}{r}$ after substituting the limits and then left hand side we should be having $\ln(1 + x_{A\infty})$.

Right side we will be having $-\frac{R^2 N_{A0}}{c D_{AB}} \left(\frac{1}{r}\right)$. So, r^2 and then that r must be cancelled out. So, then we have only $-\frac{RN_{A0}}{c D_{AB}}$ right. So, now, here what we get? $N_{A0} = \frac{-c D_{AB}}{R} \ln(1 + x_{A\infty})$. So, this equation is in final form and then usable form because c would be known for a given system D_{AB} would be known for a given system a priory and then radius of the particle is known initial part right.

So, $\ln(1 + x_{A\infty})$; $x_{A\infty}$ are known they are given even this R as function of t also we know alright. So, this equation is the final equation for N_{A0} . Now, once N_{A0} is known $N_{B0} \frac{dR}{dt}$ etcetera can be easily found right.

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How? We have already found that $N_{B0} = -2N_{A0}$ that equation number 5 ok. So, N_{A0} just now we found it as $\frac{-cD_{AB}}{R}\ln(1 + x_{A\infty})$. So, this you multiply by -2. So, that you will be getting $+\frac{2cD_{AB}}{R}\ln(1 + x_{A\infty})$ as N_{B0} and then R_S also we know. What is R_S ? R_S is simply N_{B0} or R_S is $-2N_{A0}$ which is same as equation number 8. So, equation number 8 and then 9 are same.

One is indicating N_{B0} another indicating R_S , but both of them are equal to each other for this problem right and then $\frac{dR}{dt}$ we found $-\frac{R_S}{C_C}$ from equation number 5 right. So, that we have already derived. So, here R_S is nothing, but $-2N_{A0}$ from this equation that is $\frac{2cD_{AB}}{R}\ln(1 + x_{A\infty})$ and divided by C_C is there and then this minus is there right. So, that is $\frac{dR}{dt}$. So, we got all the quantities.

And did flux rate of reaction $\frac{dR}{dt}$ all of them are interrelated now ok. So, we can find out if we know the size of the particle and then power stream conditions then we can find out whatever we want. So, second part of the problem also completed.

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$$e = 4x \ 4y \ 4z$$
C) Relate the heat flux and reaction rate at the particle
• Interfacial energy balance (neglecting radiation)
• $\left(e_r - \sum_i C_i \overline{H}_i \frac{dR}{dt}\right)_{R^+} = \left(e_r - \sum_i C_i \overline{H}_i \frac{dR}{dt}\right)_{R^-}$
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Now, third part of the problem relate the heat flux and then reaction rate at the particle; at the particle that is again at the interface. So, interfacial energy balance if you do, we are not taking any radiation which may be possible in general in such kind of combustion problem, but we are not taking. So, the balance equation we do $\left(e_r - \sum_i C_i \overline{H}_i \frac{dR}{dt}\right)|_{R^+}$ that is towards the gases stream side = $\left(e_r - \sum_i C_i \overline{H}_i \frac{dR}{dt}\right)|_{R^-}$ that is towards the particle side.

Now, you may be asking, why you are writing e_r why 0 just e? Because like in a Cartesian coordinate we have solved one problem and this derivation also we have done. So, this e is having components e_x , e_y , e_z likewise in this problem also in spherical coordinates e_r , e_θ ,

 e_{ϕ} are there, but in θ and ϕ direction no heat transfer is taking place according to this condition given.

So, we have only e_r component. So, that is the reason only e_r we are writing right and then this again includes the contribution of conduction, convection, work done due to the pressure and then viscous stress or a you know viscous dissipation terms etcetera all other terms are included here except the reaction and then mass flux part. So, those how to bring those mass flux parts in this e_r or e_x we have seen previously in one of the problem similar way that we are going to write for this case also.

So, e_r is nothing, but q_0 that is conduction part because in this problem only conduction is taking place according to the problem statement and then conditions given in the problem statement and then heat associated with the mass transfer part is nothing, but this part that is $N_{A0}\overline{H}_A + N_{B0}\overline{H}_B + N_{C0}\overline{H}_C - (C_{A0}\overline{H}_{A0} + C_{B0}\overline{H}_{B0} + C_{C0}\overline{H}_C)\frac{dR}{dt}$ this is because of the reaction part.

And then change of a particle size that should be balanced wise similar things would also be there for e_r in the particle size or R^- that is towards the particles right towards the particle the penetration of a species are not taking place gaseous species are not penetrating into the interior of the particle. Moment they come oxygen is coming immediately reacting carbon monoxide is forming immediately it is diffusing back to the bulk gases stream.

So, no gases stream are going inside the particle and then no heat conduction is taking place inside the particle whatever the heat transfer is taking place from the surface to the bulk of the gases stream only taking place. So, all the terms are negligible right. So, this q_0 and then $N_{A0}N_{B0}N_{C0}$ all those terms are negligible towards the particle size only thing is say that is $C_C \overline{H}_C \frac{dR}{dt}$.

 C_C is the concentration of the carbon particle, \overline{H}_C is that molar enthalpy of that carbon particle and then $\frac{dR}{dt}$ is that change in the size of the particle with respect to the time because of the reaction. So, now, we simplify this equation. So, q_0 would be there towards the gases side N_{A0} there is something just now we derived an expression, N_{B0} is also there just now we derived an expression. But, towards the gases stream the carbon is not there, carbon is there only in the interior of the particle from the surface to the interior only that part only carbon is there from the surface it is reacting and then forming carbon monoxide. So, gases stream no carbon is there so then this term is 0 right. Now, coming to this part what we have? C_{A0} . C_{A0} is what? It is a concentration of oxygen at the surface right at the surface though it is towards the gas, but whatever the oxygen is there that is immediately being consumed by the carbon for the combustion reaction so this is not there.

 C_{B0} would be there because immediately after a reaction between carbon and oxygen carbon monoxide is forming. So, it must be having some concentration that is designated by B. So, C_{B0} would be there. Then again C_{C0} is nothing, but the concentration of carbon towards the gases side it is not there; towards the gas side it is not there because it is there only towards the particle side, towards the gaseous side only oxygen and carbon monoxide are there.

So, then what we are having $q_0 + N_{A0}\overline{H}_A + N_{B0}\overline{H}_B - (C_{B0}\overline{H}_B)\frac{dR}{dt} = -C_C\overline{H}_C\frac{dR}{dt}$ right. So, the same equation is written here once again right.





But, whatever N_{A0} ; N_{A0} was nothing, but $-\frac{R_S}{2}$ from equation number 5 and then N_{B0} is nothing, but simply R_S and then this $\frac{dR}{dt}$ is nothing, but $-\frac{R_S}{C_C}$ from equation number 5. So,

that we have written. So, same thing in the right hand side also in place of $\frac{dR}{dt}$, $\left(-\frac{R_S}{C_C}\right)$ we have written ok.

Refer equations 4 and 5 for this transformation in terms of R_S ok. So, q_0 what we are doing? We are combining this term and then this term and this term and then writing $R_S\left(\frac{-\overline{H}_A}{2} + \overline{H}_B - \overline{H}_C\right)$ because here this C_C this C_C is already cancelled out and then this remaining term is nothing, but $+ \frac{C_{B0}\overline{H}_B}{C_C}R_S = 0.$

And now this is nothing, but this is nothing, but ΔH_R for the entire reaction, A enthalpy associated with the reactants and then C is also associated with the reactants and then B is associated with the product enthalpy. So, this is for the overall reaction. So, that is $q_0 + R_S |\Delta H_R + \frac{C_{B0}\overline{H}_B}{C_C}R_S = 0$. So, now, this equation you have to solve to get this q_0 because the part of the question is that one only, we have to find out heat flux at particle surface that is q_0 .

So, this equation you know if you can solve you can get this q_0 , but that is not possible unless and until you know some kind of information between this two. So, what we assume that this ΔH_R is much higher compare to the $\frac{C_{B0}\overline{H}_B}{C_C}$ or $\frac{C_{B0}\overline{H}_B}{C_C}$ is very very smaller than the ΔH_R and then use Fourier's law of conduction for q_0 then you can solve this equation.

Because in general ΔH_R of the reaction you can know they are provided R from the thermodynamics or reaction kinetics of non-isothermal reactions we can find out. So, that should not be a deal ok and then this should also be making sense because compared to the concentration of the carbon, concentration of carbon monoxide is very small at the interface. So, this ratio is going to be very small close to 0 as we already seen.

So, the overall when it is multiplied by \overline{H}_B it is going to be very small compared to you know heat of the reaction that is ΔH_R ok. So, q_0 we can write $-k_G \frac{dT}{dr}|_{R^+} = -R\Delta H_R$. So, now, this equation you can solve right, only thing that you need to know what is $\frac{dT}{dr}$ and all that. G we are writing just to indicate that is towards the gaseous side whatever the conduction is there towards the gaseous side. Otherwise, we may be confusing with k of a carbon particle ok, this is all we are doing towards the gaseous side.

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So, that was the part three that is finding the heat flux at the surface ok. If you know the heat of the reaction and then $R_S C_C$ you can find out that particular q_0 at the surface ok. Now, determining the particle temperature T_0 we have to find out. Particle temperature at the surface whatever is there that we are designating as T_0 .

So, what we do now for this purpose? We will be writing energy conservation in the gas. So, what we got $\frac{\partial}{\partial r}(r^2 e_r) = 0$ that we already got which is pseudo steady, spherically symmetric case. So, this we got it as $(r^2 e_r) = f(t)$ ok constant and that constant is function of time it is independent of r, but function of time. So, we can write $e_r = \frac{f(t)}{r^2}$ and then e_r is having the conduction part and then mass transfer part $= \frac{f(t)}{r^2}$.

So, here N_{Cr} is anyways 0, N_{Ar} is nothing, but you know we got $N_{A0} \frac{R^2}{r^2} \overline{H}_A$ is as it is N_{Br} is nothing, but $-2N_{Ar}$. So, $-2N_{Ar}$ is again $N_{A0} \frac{R^2}{r^2} \overline{H}_B = \frac{f(t)}{r^2}$, q_0 is simply $-k_G \frac{\partial T}{\partial r}$ ok. So, this equation further we can write by taking $N_{A0} \frac{R^2}{r^2}$ as common. So, the remaining terms are these two right. This equation what we do? We divide both sides by $-k_G$.

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That dividing we will do later the same equation is given here now. Now, what we do? We have to take some reference temperature in order to define these things this $\overline{H}_A \ \overline{H}_B$ usually defined with respect to some reference temperature. So, that we can write you know we can bring in \overline{C}_{PA} , \overline{C}_{PB} , ΔT etcetera. Because, \overline{C}_{PA} , \overline{C}_{PB} , information are known for many of the cases in general ok from the standard thermodynamic books.

So, assume that \overline{H}_i is nothing, but $\overline{H}_i^* + \overline{C}_{pi} \Delta T$, ΔT is nothing, but $T - T^*$; T^* is some reference temperature let us assume. So, that this equation we can write $-k_G \frac{\partial T}{\partial r} + N_{A0} \frac{R^2}{r^2} (\overline{H}_A^* - 2\overline{H}_B^*) + [\overline{C}_{PA} - 2\overline{C}_{PB}] \Delta T$ that is $T - T^*$, this ΔT is only for this $[\overline{C}_{PA} - 2\overline{C}_{PB}] = \frac{f(t)}{r^2}$ is as it is.

So, now, this equation what we are doing? Dividing by $-k_G$ both sides to get this equation. So, that is $\frac{\partial T}{\partial r} - N_{A0} \frac{R^2}{k_G r^2} [\bar{C}_{PA} - 2\bar{C}_{PB}](T - T^*) = \frac{g(t)R^2}{r^2}$ we are writing right. So, this whatever term is there this term is combined together and written as like this.

So, $\frac{g(t)R}{r^2}$ is nothing, but $\frac{f(t)}{k_G r^2} + N_{A0} \frac{R^2}{k_G r^2} \left(\overline{H}_A^* - 2\overline{H}_B^*\right)$ right ok. So, now, this f (t) functions they are not mixed r^2 they are written, but they are not combined they are separately there. So, we can integrate them later anyway.

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$$\begin{array}{l} \cdot \Rightarrow \frac{\partial T}{\partial r} - \underbrace{N_{A0}R^2}_{k_G f^2} [\bar{C}_{PA} - 2\bar{C}_{PB}] (T - T^*) = \frac{g(t)R}{r^2} \rightarrow (12) \\ \cdot \text{ Now let, } T^* = T_0 \text{ (surface temperature) and} \\ \cdot \eta = \frac{r}{R} \hspace{0.2cm} ; \hspace{0.2cm} \theta = T - T_0 \hspace{0.2cm} ; \hspace{0.2cm} \Lambda = \frac{N_{A0}R}{k_G} (\bar{C}_{PA} - 2\bar{C}_{PB}) \hspace{0.2cm} \text{so that eq. (12)} \\ \text{ becomes} \\ \cdot \frac{\partial \theta}{R\partial \eta} - \Lambda \frac{R}{\eta^2 R^2} \theta = \frac{g(t)R}{R^2 \eta^2} \Rightarrow \frac{\partial \theta}{\partial \eta} - \frac{A\theta}{\eta^2} = \frac{g(t)}{\eta^2} \rightarrow (13) \\ \cdot \text{ and } \theta = 0 \hspace{0.2cm} \text{at } \eta = 1 \\ \cdot \text{ To find out } T_{\theta} \text{ we must evaluate } \theta(\infty, t) = T_{\infty} - T_{0} \end{array}$$

So, finally, this is the same equation we have written here. Now, let that reference temperature $T^* = T_0$ so that this equation we can solve. Further what we are doing that $T - T_0$ we are taking as Θ right in order to do the non-dimensionalization. And then $\frac{r}{R}$ we are taking η and then whatever this constant $\frac{N_{A0}R}{k_G} [\bar{C}_{PA} - 2\bar{C}_{PB}]$ is there that we are calling Λ .

So, that this equation number 12 will become $\frac{\partial \Theta}{R \partial \eta} - \Lambda \frac{R}{\eta^2 R^2} \Theta$ would be there, this only here this you know this entire thing except this r^2 whatever the terms are there this entire thing is nothing but Λ except this r^2 were in the Λ we are not having the square term. So, that is the reason this R is coming here and then r^2 is nothing, but $\eta^2 R^2 \Delta T$ is nothing but Θ , = $\frac{g(t)R}{\eta^2 R^2}$.

So, squares, so that $\frac{\partial \theta}{\partial \eta} - \frac{\Lambda \Theta}{\eta^2} = \frac{g(t)}{\eta^2}$. So, at $\eta = 1 \Theta = 0$ to find out T_0 we must evaluate Θ as function of location $r = \infty$ and time that is $T_{\infty} - T_0$, because T_{∞} is known right. So, this equation if you solve in at $r = \infty$ you can find out what is this T_0 . So, that we are going to do.

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So, the equation is written here once again and it is in the form $\frac{dy}{dx} + p(x)y = q(x)$; p and q are functions of x. So, its solution is that y (IF) $= \int q(x)(IF)dx$ where (IF) is nothing, but $e^{\int p(x)dx}$. So, here p is nothing, but $-\Lambda/\eta^2$ and then $q = \frac{g(t)}{\eta^2}$. Hence integration factor would be $e^{\int (-\Lambda/\eta^2)d\eta} = e^{\Lambda/\eta}$.

And then solution would be Θ multiplied by this I F is $\Theta e^{\Lambda/\eta} = \int \frac{g(t)}{\eta^2} e^{\Lambda/\eta} d\eta + h(t)$ multiplied by I F integration with respect to $d\eta$ + integration constant which is again function of time. Now, we got another integration constant which is function of time which is constant with respect to r. (Refer Slide Time: 56:02)



So, that equation further if you solve right hand side integration. So, then you have this equation. So, that $e^{\Lambda/\eta}$ if you take to the right hand side, so this Θ is nothing, but this one right. So, next part what we are doing? We are writing h (t) $e^{-\Lambda/\eta} - \frac{g(t)}{\Lambda}$ because this and this exponential of one is + and another one is minus. So, then exponential of 0 is 1.

So, this is the temperature distribution as function of a r and t, but it is written in dimensionless form, but this equation we can only use when we know what is this h (t) and g (t) right. So, but here if you substitute boundary condition $\eta = 1$, $\eta = 1$; that means, r = R at r = R, $T = T_0$. So, Θ is nothing, but T - T₀, so that should be 0. So, Θ (1, t) should be 0 *h* (*t*) e^{-A} should be equals to $\frac{g(t)}{A}$.

So, that in place of $\frac{g(t)}{\Lambda}$ we can write h(t) $e^{-\Lambda}$. So, that we write and then take h (t) common. So, we have h (t) function of $e^{-\Lambda/\eta} - e^{-\Lambda}$. So, then we have this equation. So, it is better compared to this equation, but still there is a h (t) without this one we cannot use this equation.

So, now we have to evaluate this h (t) from this interfacial energy balance what we got? $q_0 = -k_G \frac{\partial T}{\partial r}|_{R^+} = -R_S \Delta H_R$ so; that means, $\frac{\partial T}{\partial r} = \frac{R_S \Delta H_R}{k_G}$ this equation we non-dimensionalize. (Refer Slide Time: 58:28)



So, this equation same written here if we non-dimensionalize then we have $\frac{\partial \Theta}{R\partial \eta} = \frac{R_S \Delta H_R}{k_G}$ that R of left-hand side we bring to the right hand side. And then substitute $\eta = 1$ because we are doing at r = R. So, at r = R $\eta = 1$. So, that is a constant actually. So, that Γ we are calling right. Now, equation 14 this is what we have. We will differentiate this equation also with respect to η and then substitute $\eta = 1$.

So, by differentiating with respect to eta this is what we have. And then substituting η i=1 this is what we have. So, that these two equations you can compare and then have an expression for h (t). So, h (t) would be $\frac{\Gamma e^{\Lambda}}{\Lambda}$ right this is what we have. This now you can substitute in equation number 15. So, that you have the temperature profile this part is nothing, but your h (t). So, we got through came over this h (t) as well.

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So, next step what we do? $e^{-\Lambda}$ we bring in inside the parenthesis. So, that we have this one right. Now, we wanted to measure the temperature at ∞ location actually Θ is nothing but $T - T_0$. So, $-\Theta$ would be $T_0 - T$ and then if you evaluating this Θ at ∞ that T should be T_{∞} . So, $T_0 - T_{\infty}$ would be minus of this one, so this one.

And then η is ∞ , so $\frac{1}{\eta}$ is 0, so this part is then here. So, $T_0 - T_{\infty}$ is nothing, but this all expression from here we can get final T_0 expression T_0 is nothing but T_{∞} minus this expression. But, Λ is very very less than 1 that is particle is very small in general then $e^{\Lambda - 1}$ is approximately Λ .

So, that we can have $T - T_{\infty}$ = minus simply Λ . So, then this is what the expression. So, this is the overall general solution this is the solution when particle size is very small for the surface temperature ok.

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So, references for this problem are provided here, but this problem is taken from this reference book.

Thank you.