

**Microscale Transport Processes**  
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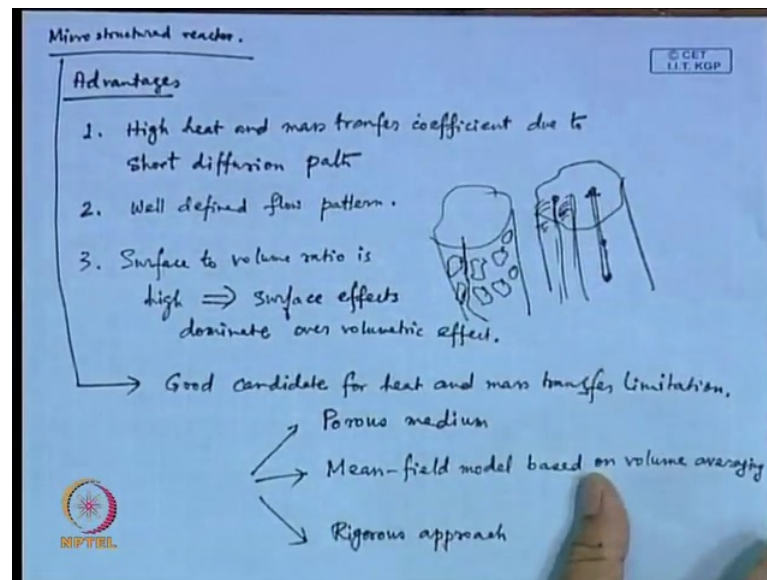
**Module No. # 01**  
**Lecture No. # 28**  
**Microstructured Reactor**

I welcome you to this lecture of micro scale transport process, what I wanted to talk about today is microstructured reactor. So far we have covered several aspects of micro scale transport process, particularly this electro kinetic phenomenon, like electro osmosis, di electrophoresis and topics like that. Also I talked about this slip flow, which is more important for **for** flow of a gas and how this first order slip boundary condition can be handled in a micro couette and micro poiseuille flow that I discussed in the last class.

In this class, I briefly I will touch upon certain issues of modelling a microstructured reactor, **as there are certain** there are certain aspects of microstructured reactor there are certain assumptions that can be made for a microstructured reactor, these **these** assumptions would help simplifying the problem otherwise, you can always solve a problem from first principle. And write a very detailed CFD model however, when it comes to solving it quickly, when it comes to solve have a simplified model, I would like to talk about those assumptions that can be made for a microstructured reactor.

I hope I will be able to finish this topic today, and from next class I will be discussing about transport of or flow of immiscible phases, that means two phases simultaneously flowing through a micro channel. So, this class I will be talking about some aspects, how we can simplify the design of or **or** the modelling of a micro structured reactor.

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Now, let me point out that this microstructured reactor, the reason why we have gotten into this micro structured reactor is, that the reason we have gotten into this microstructured reactor is that, you have certain advantages. The advantages are advantages are number one high heat and mass transfer coefficient due to short diffusion path.

Number two is well defined flow pattern, why I mention this well defined flow pattern is that, the other candidate that could I mean if you if you look at other modes of in other mode by which these reactors operate in on an industrial scale, is basically packed bed type reactor. But, inside a packed bed the the channels are pretty random, that means in some places channels are wider and in some places channels are too constricted, so the flow pattern is not well defined.

And if the flow pattern is not well defined, you do not know what type of what type of heat transfer mode or mass transfer mode would be working there, and more more importantly it could be that some places. Inside this pack bed in some places the weight of or or the amount of catalyst studies available per volume of per volume of influent is much higher and in some places it is much lower.

So, having a control over the conversion, having a control over the side reactions or having a control over the heat of reaction that that it that is generated or heat of reaction that is observed. So, that control becomes difficult, if you have that random path ways,

so here in this case you have well defined flow pattern, that means what I mean you remember, how we described these microchannel reactor these **these** are basically a very structured, honeycomb type structure. So, you **you** have a monolith that means, **you** have **have** you seen a honeycomb, you have a monolith and **and** in that you have channels engraved; so these channels are running parallel.

But, these channels are very **very** well defined that means, the **the** aperture here or the cross section here and the cross section here and the cross section here they are same, so you have a monolith and you have these channels running (Refer Slide Time: 05:02). So, **so** basically you first **I mean if you** if you ask me how do you generate this, basically you have monolith first and then you wash coat it, that means you **you you** apply a coating of catalyst on the wall of these channels, so that is how you generate **these** these catalyst monolith.

And now you have flow going through these channels, in case of **(())**, in case of a packed bed what you have is, you have the same packed bed only thing is you have those catalyst pellets here, and the flow was ask **flow was** flow was forced through these constructions. So, in some places channels are wider, some places channels are **(())**, so that is what I said first of all the flow pattern is not well defined, so you do not know in which regime you are working, and also you do not know, what would be the catalyst that this flow encounters per unit volume.

And that probably defines **how how much** how fast the reaction would be or whether there should be any side reaction or not, and if there is too much of reaction then what you want, there could be a possibility of thermal run away. That means, there would be **if it is** if it is exothermic reaction and too much of heat gets generated that you that you do not have any procedure to control, then the catalyst would be spoiled by **by** that heat. So, these problems are there, so in **in** case of microstructured reactor **you can** you can get rid of this, anyway **these are** these are some of the issues that would be have, we already know probably.

Number 3 is that surface to volume ratio is high, so what this implies is **surface effects** surface effects dominate over volumetric effect. So, because of these advantages you have these basically, these microstructured reactor, these are **good candidates** good candidate for heat and mass transfer limitation. Think of a reaction which is highly exothermic

or highly endothermic and you need to precisely, you need to run that reaction at a precise temperature; so in that case having that control in a packed bed is not easy however, this microstructured reactor that promises that **it can be** it can be done in a better way.

Now, what we **we** must say here is that, this when it comes to modeling these **I mean** of course, you can say that **we can** we can do it **in a** in a, using the standard **the** theories that are available for CFD, **that is** that is in fact, the way of doing it, the rigorous way of doing it. However, we are looking for some assumptions that can be made such that, the some simplified approach can be developed.

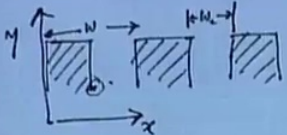
Now, when it comes to developing a simplified approach, I see there are basically three approaches possible, one is treat this microstructured reactor as a porous medium, second is use something called a mean field model based on volume averaging **based on volume averaging** and the third is the rigorous approach **third is the rigorous approach**.

So, this is actually, this is going to be the simplest one, the porous medium based model this is somewhat complicated, but it does not take care of all **the I mean it it** still it make some assumptions; and the third one is the rigorous approach which you should be doing. Treating the two fluids and the Navier solving, Navier-Stokes and heat balance and mass balance equation over a differential element, the way we do it for a standard fluid, standard flow reactive flow problem.

Now, what is this porous medium model, porous medium, so these channels I said that it is like a honeycomb **it is it is like a honeycomb**, so you have these channels which are running along the length of the reactor. Rest of **rest of** the matrix is what solid, these are solid material and in that you have channels running.

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Porous Medium



Incoming flow is distributed over large number of channels of width  $w_c$ , separated by walls with a width of  $w - w_c$ .

$$\frac{d}{dy} \langle P \rangle_f + \epsilon \frac{\mu}{k} \langle u \rangle_f = 0$$

where  $\epsilon = \text{porosity} = \frac{w_c}{W}$

$$k = \frac{\epsilon w_c^2}{12} \quad \text{Cubic law.}$$

$P \equiv \text{pressure}$   
 $u \equiv \text{velocity.}$   
 $\langle \rangle_f$  represents average over fluid phase.

$$\rightarrow (1 - \epsilon) c_s \rho_s \frac{\partial T(x, y, z)}{\partial t} + \rho_f c_f u \frac{\partial T}{\partial y} = \lambda \frac{\partial^2 T}{\partial y^2} + \text{Heat of rxn.} \quad \text{-- closes, if any.}$$

Now, if you want to treat this as a porous medium, then what you would be doing is let me draw this how **how** it will appear, this is the solid part, this is the open part through which the flow can pass, again this is the solid part, again some open portion, then again there is a solid part and this open portion (Refer Slide Time: 10:50). Suppose this direction is x, this direction is y and this distance is w whereas, this distance is  $w_c$ , one is the channel and the other is channel plus the solid part **alright**, so you have a series of this, not just 3, 1000s of them.

Now, **what we what we** what we must say here is that, the incoming flow **incoming flow** is distributed over large number of channels of width  $w_c$ , separated by walls with a width of  $w$  minus  $w_c$ . So, there are walls, the width of the wall is  $w$  minus  $w_c$  and width of the channel is  $w_c$  **this is this is** this I think, this should be this is understandable.

Now, I think you are familiar with **with** a theory called Darcy's law **if we** if we apply that it would appear like this,  $\frac{d}{dy} \langle P \rangle_f + \epsilon \frac{\mu}{k} \langle u \rangle_f = 0$ , where  $\epsilon$  is equal to so called porosity, which is  $w_c$  by  $w$ , basically you have another **another another** dimension added to it. Basically, porosity is considered volume by volume, volume of wide divided by the total volume, so here you have only one dimension you are considering, so other two dimensions needs to be multiplied to this.

So, **you are** you are considering that **this** these two dimensions would be multiplied in the numerator and denominator they just cancelled out, and  $k$  typically **this is for a** this is

considered (O) for a porous flow through porous medium. Now, this has been this has been shown that when you have a channel and if you want to find a permeability for a flow through by channel, there is a there is an expression available, when you have two flow between flow between two parallel plates, two parallel walls.

And that that the flow through that channel which made by two parallel walls, you can come up with an expression for k and that expression is given by  $\epsilon \rho a w c^2$  divided by 12, that is that is how it is given (No audio from 14:40 to 14:48) or what you can do is, I mean if you (No audio from 14:51 to 15:03) well this is this is the expression this is this expression has been obtained by one one researcher in in in sometime back.

This is this later on this this one one researcher from from university California Barclay he first in (O) he proposed this expression, I mean that is what I hope I am I mean I remember, that is what I remember, and later on this was referred as cubic law, so this is this is this is how this permeability can be defined for a flow through a channel.

Now, you you can you can, let me let me point out couple of things here before I go for that, p here is pressure, u here is a velocity and this quantity something in this kind of bracket with f written as a subscript. This represents average over fluid phase average over fluid phase alright, so this is this is how this pressure and velocity they can be related, if you consider this to be a porous medium.

Now, let me write the full form in what what all we are doing here, the other issue is here the heat transfer, which is written as  $1 - \epsilon \rho a c s \rho \Delta T \Delta t + c g \rho g u \bar{\Delta T} \Delta x$  that is equal to  $\lambda \Delta^2 T \Delta x^2$  plus heat of reaction minus losses if any. This I am saying this is this is this is how it is considered the heat transfer, the heat balance equation what are you doing here, I mean can you can can can somebody guess what what are we up to, why I mean, what is prompting us to write it (O).

We are talking about only one temperature, have you noticed that, whose temperature is this then, I am talking about a monolith, I am talking about some portions are solid material, then I have a coating of catalyst on the wall which is helping me achieving the whatever conversion that I want to achieve.

And I have a flow going on through this channels, whose temperature is this now and how are we writing this, so that could be **I mean that that is** that is **(())** the assumption, you are treating this to be as if it is a single medium. And it has temperature **I mean** I have temperature as a function of time, temperature as a function of x I can see or **or should it be should it** should it be  $\lambda$ , this should be  $\frac{\partial}{\partial y}$ , we have considered this direction, so flow is going on this directions, so actually we are looking at  $\frac{\partial T}{\partial t} \frac{\partial T}{\partial y}$  here.

So, in that case this should be y not x, so **we are** we are considering this temperature as a function of time and position, that much is understood however, you are considering only one temperature, so at **at** least and what you how treating this medium is achieved this medium **is just** this just a homogeneous bed. And in that temperature is just at **at** one point, the temperature there is only one temperature that means, whether it is a fluid temperature or solid temperature you are assuming that they have equilibrated.

These two say a fluid at this point and the solid nearby they are all equilibrated, there **(())** any difference in the temperature of fluid and solid, say **say** we are talking about a point here **here a point** here the solid temperature and fluid temperature you are not differentiating it. You are treating it **I mean** you are giving the temperature a function in position, temperature is a function of time.

But, solid and gas you are not separating you are considering only one temperature you are considering that the solid and gas they are in equilibrium, inside the medium. So, that means, fluid is flowing say **as as as this travel** as this travels on the bottom to top, fluid is flowing, so at any point the fluid and the solid temperature there, they are considered same, that is how this **this** equation is to be solved.

It **it** is this **this** is possible when the channel dimension is really small, this **this** type of assumption is considered in porous medium, when the channel dimension is small and the gas is flowing through that channel. So, in a microscopic sense you can consider that the gas and the solid at that point these two temperatures are same; they are equilibrated. This is of course, not a rigorous approach that is what I say, this is an assumption, so **what you** what you write, **I mean** I should be writing here.



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large number of channels of width  $w_c$ , separated by walls with a width of  $w-w_c$

$$\frac{d}{dy} \langle P \rangle_f + \epsilon \frac{\mu}{k} \langle u \rangle_f = 0$$

where  $\epsilon = \text{porosity} = \frac{w_c \cdot N}{w}$

$$k = \frac{\epsilon w_c^2}{12} \quad \text{Cubic law.}$$

$\langle \rangle_f$  represents average over fluid phase.

$$\rightarrow (1-\epsilon) C_s \rho_s \frac{\partial T}{\partial t} + \rho_s u \frac{\partial T}{\partial y} = \lambda \frac{\partial T}{\partial y} + \text{Heat of con. if any.}$$

Above equation assumes thermal equilibrium between the fluid and solid phase. Single temp. field is used for fluid and solid phase. At large Pe No., this assumption breaks down.

In this case is that above equation assumes above equation assumes thermal equilibrium thermal equilibrium between the fluid and solid phase, single temperature single temperature field you remember, velocity field, velocity depends on position and time, so single temperature field is used for fluid and solid phase fluid and solid fluid and solid phase; this assumption is this is told that these assumption breaks down at high (Pe) number at large (Pe) number this assumption breaks down alright.

Now, so you you understood what, how how we have approach this porous medium problem, I mean let me recapitulate once again, let me repeat we have come up we we said that it is the, we we have define  $w_c$  and  $w$  is obvious. And the and if you add another dimension to it, porosity can be defined by  $w_c$  by  $w$  basically other two dimensions need to be multiplied to the numerator and denominator, they have cancelled out.

This basically, porosity defined as the volume of wide divided by that total volume, there is an expression for permeability which you can this this you can you can you can check in the Darcy's law, which is which is which has been there for quite some time. This Darcy's law it is basically, this this will come directly from there. And this permeability term which is this Darcy's law typically used for porous medium, however that same equation can be applied for a flow through a channel, where permeability can be given as this quantity, aperture of the channel to the power square divided by 12, so



that is how you **you** define and **this is** this is referred as cubic law. And here in this expression I am mentioned  $p$  as pressure, and  $u$  as velocity and this quantity within bracket, with a subscript  $f$  these represents average over fluid phase; that means, we are talking about  $u_f$  this is average over the fluid phase, we are not within a fluid phase we are not differentiating layer by layer or any **any** profile we are not adding here, velocity profile or anything.

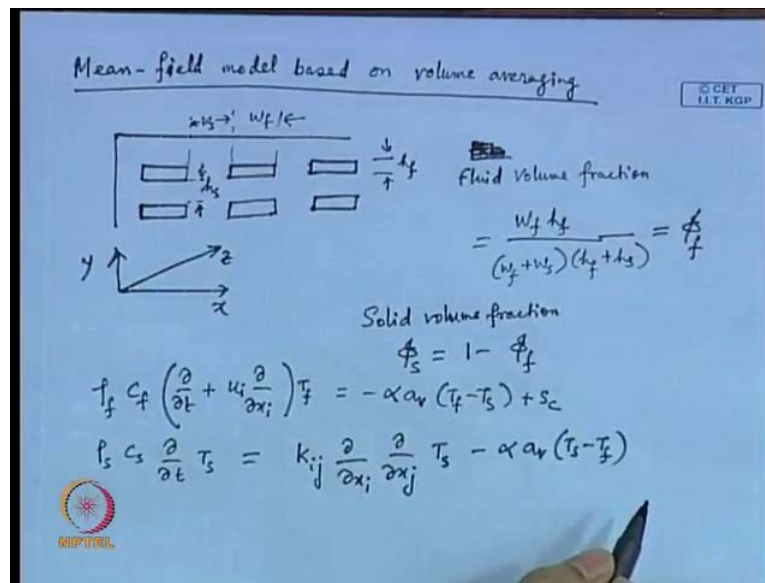
Now, you come up with that temperature at the heat balance equation ideally you should have two temperatures, one for the fluid another for the solid, and the fluid temperature should have a profile within the channel. So, their temperature would be maximum or **or** depends on whether it is exothermic or endothermic reaction; if it is exothermic probably that temperature would be maximum at the center of the channel.

And then at the wall it would be or as you proceed towards the wall, the temperature would be less and then there should be continuity of flux at the interphase between solid and fluid, **I mean** there are all kinds of things which needs to be considered, if you are really looking for a rigorous CFD model. However, we are looking for assumptions because, what **what** you may beask to do is to take up various dimensions of this microstructured reactor.

If **if** we change, if we take  $w$  as this  $w_c$  as this and this material with property  $c_s$  is this  $\rho_s$  is **(())**, so if you are, if you have to play with this and come up with the best design for your microstructured reactor, probably this kind of simplified model would be useful at least to **tototo screen the** screen the **thethe**, I would say the **you have a** you have a large bound to play with.

Now, if you want to come up with an optimum design, you need a simplified model first to focus on which dimensions or which material or what you need to look for, and then probably you get to the CF detailed rigorous CFD model to fine tune the results. So, **that is** that is what we are talking about, so this simplify model is meant **for fora** for a particular purpose, and by now you must have understood the purpose.

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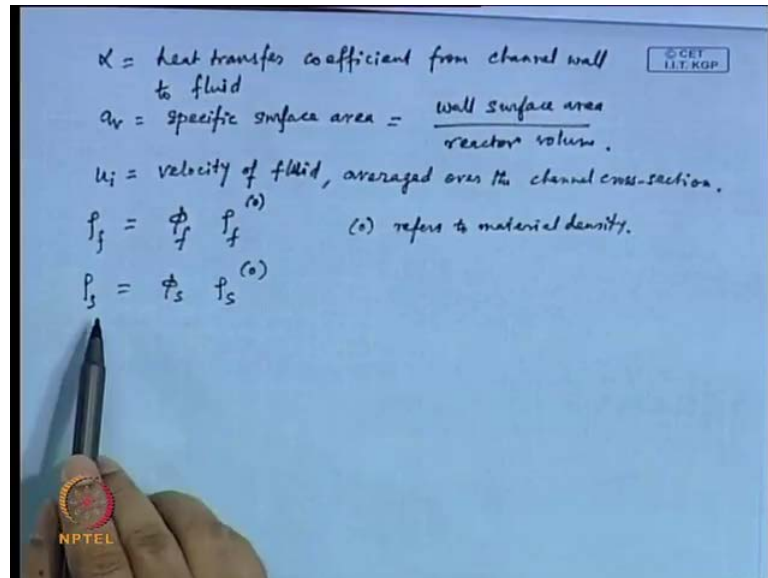
Now, you you we what we have here is, the next topic is this, so this this is porous medium, this is the most simple model that I have, that I had to talk about; the second model is mean field model based on volume averaging mean field model based on volume averaging. What you do here is, if you have (No audio from 26:57 to 27:17) (Refer Slide Time: 26:57) this distance is  $w_f$ , and this distance is  $w_s$  similarly, this distance is considered  $h_f$ , and this distance is considered  $h_s$ .

And you are considering  $x$  in this direction, and  $y$  in this direction and  $z$  in direction perpendicular to the paper, so flow is taking place perpendicular to the paper through these channels alright. Now, if you need to find out what is the phase volume fraction, that means, what is the fluid volume fraction in these in these in this reactor; so if I call this phase volume fraction or let us let us call this fluid volume fraction, and there are two volume fractions, one is fluid and other is solid.

So, fluid volume fraction that is equal to  $w_f h_f$  divided by  $w_f h_f + w_s h_s$  alright, this is how you define the fluid volume fraction, and this we call is equal to  $\phi_f$  and then the solid volume fraction, that is  $\phi_s$  which is equal to  $1 - \phi_f$ . Now, if you try to write the heat balance equation, this will take the shape, I mean here what we will be doing is we will be treating the temperature of fluid and solid separately; but, it will not be fully it will not be full rigorous model. So, the heat balance equation would be  $\rho_f c_f \frac{\partial}{\partial t} T_f + u_i \frac{\partial}{\partial x_i} T_f = -\alpha_{av} (T_f - T_s) + s_c$

minus  $T_s$  plus  $s_c$ ,  $s_c$  is a generation term, generation from reaction term. For the solid you have  $\text{del del } T$  of  $T_s$  no convection possible within the solid, and that is given by **some the** some conductivity tensor, thermal tensor and that is  $\text{del del } x_i \text{ del del } x_j$  of  $T_s$  minus  $\alpha a_v T_s$  minus  $T_f$ , this is how you want to write this expression.

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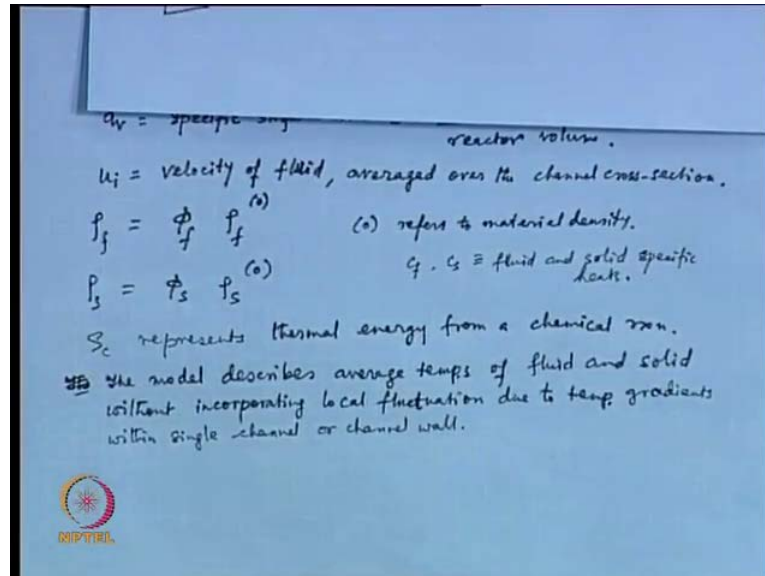
Now, **let me** let me clarify the meaning of various terms, **I will** I will use another page and I will come back to this expression, so after I define all these terms, here **here**  $\alpha$  is equal to heat transfer coefficient from channel wall to fluid, and  $a_v$  is equal to specific surface area; that is equal to wall surface area divided by reactor volume.  $u_i$  is equal to velocity of fluid, averaged over the channel cross section (No audio from 32:13 to 32:23).

Here,  $\rho_f$  is equal to  $\phi_f \rho_f^{(s)}$ ,  $\rho_f^{(s)}$  is basically **this** subscript 0 refers to **material densities** material density, because you are talking about a  $\rho_f$ , so this  $\rho_f$  as far as this bed is concerned this has to be multiplied by the **(phi)** volume fraction or the phase fraction of the fluid, then you get the actual  $\rho_f$  which should be applicable for this.

Here, we are working on a mixed model **I mean it is it is not** it is not very straightforward **you need** you need to look into it very critically, we have this as  $\rho_s^{(s)}$ , this 0 refers to material density, so  $\rho_s$  is equal to, **so the** so if we, so think of it we have a  $\rho_f$  here, we have a  $\rho_s$  here, but this  $\rho_f$  and  $\rho_s$  they are not the density of the solid and

density of the fluid. Rather, they are pure component density of the solid multiplied by the corresponding void fraction, how much solid what fraction the solid is occupying within the bed, so that so that so then only we can make this, we can do this treatment.

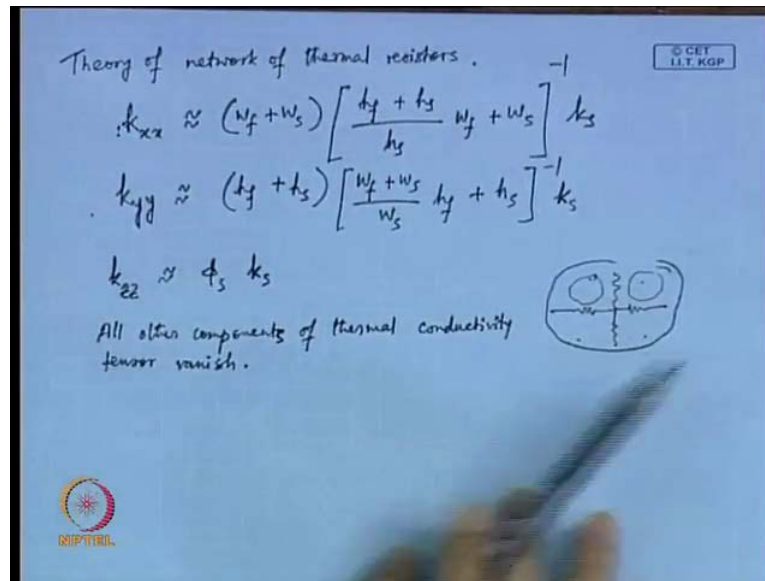
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$S_c$  represents  $S_c$  represents thermal energy from a chemical reaction, and this model describes the model describes of course, we we have to define to this  $c_f$  and  $c_s$   $c_f$  and  $c_s$  they are fluid and solid fluid and solid specific heats; so the model describes average temperatures of fluid and solid, without incorporating local fluctuation due to temperature gradients temperature gradients within single channel or channel wall.

Then now, the question would be how you handle this  $k_{ij}$  this term, how will you get  $k_{ij}$ , so this is not neither a property of the, neither the thermal conductivity of the solid material, it cannot be treated that way (Refer Slide Time: 35:40). So, the what researches have done is they have come up with, they have used something called a theory of network of thermal resistors.

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It is a network of thermal resistors and what they have done is they have obtained  $k_{xx}$  as  $w_f + w_s$  into  $h_f + h_s$  divided by  $h_s$  into  $w_f + w_s$  inverse into  $k_s$ .  $k_{yy}$  this is equal to  $h_f + h_s$  into  $w_f + w_s$  divided by  $w_s$  into  $h_f + h_s$ , and  $k_{zz} = \phi_s k_s$ ; this follows from theory of network of thermal resistors.

So, if you here you have thermal resistors, but **how is it** how is it aligned **I mean** think **think** in that line, how is it aligned you have one channel, then you have another, **I mean** think of it there is one channel then this is connected to another channel in this direction, this is connected to another channel in this direction, this is connected to another channel (Refer Slide Time: 37:42).

And then you have those porous, the **the** void through which the gas is flowing, so you have these theory, these **these** network of thermal resistors there are certain theories and people have already researched, have already utilized those theories to come up with these expressions for  $k_{xx}$ ,  $k_{yy}$  and  $k_{zz}$ . And what, **all other components of thermal** all other components of thermal conductivity tensor vanish, because what was the equation here, this was the equation **right**.

This was the equation originally, for mean field model based on volume averaging, we have for the fluid phase  $\rho_f c_f$ , now we have already said that there was a, there is a correction for  $\rho_f$ , so  $\rho_f c_f \Delta T$ , so the you are operating this entire, you are putting this operator on the  $T_f$ , that is equal to  $-\alpha a v$ . And this is the heat

exchange term between fluid and solid, and plus some generation term similarly, for the solid you have, you do not have a convective term, so it is only the transient.

And then you have the thermal conductivity, so this is how you write and then **what you** how did we treat otherwise, it would have been  $\lambda \frac{\partial^2 T}{\partial z^2}$ , that way we **we** or  $\frac{\partial^2 T}{\partial x^2}$  or you write it as  $\lambda_x \frac{\partial^2 T}{\partial x^2} + \lambda_y \frac{\partial^2 T}{\partial y^2} + \lambda_z \frac{\partial^2 T}{\partial z^2}$  things like that. But, ideally you should be writing it, this is the most generalized way of writing it.

Now, this is the thermal conductivity tensor, what **we are with** these assumptions of mean field model and network rather more importantly the network of thermal resistors what they have come up with is that, these  $k_{xx}$ ,  $k_{yy}$ , and  $k_{zz}$  they are existing, and this is the value. And we have related  $w_f$ ,  $w_s$ ,  $h_f$ ,  $h_s$  all these things, we have come with very neat functional form here of course, I haven't the equal to sign, but approximately equal to sign.

And then multiplied by  $k_s$ ,  $k_s$  is the actual thermal conductivity, it is a bulk property **it is** it is a pure component property of the solid, so this is the pure component property of the solid, if there would not have been a channel, there would not have been a fluid passing through this solid; then we would have considered simply  $k_s$ .

But, now since, we have these channels and we have, so we **we** have now a thermal conductivity tensor, but what we are with some simplification what you came up with is that  $k_{xx}$ ,  $k_{yy}$ , and  $k_{zz}$  these are the values you have, **I mean** all other components the cross terms, all other components thermal conductivity tensor vanish. So, **now you should be** now it should **it is** it is much simpler to handle, you must appreciate this point what is the difference between a porous medium model and mean field model.

Porous medium there you did not have you just have a single temperature, porous medium model you have just one temperature, you did not differentiate between the solid and a fluid, there was just single temperature and you said they are equilibrated. Here, you are having two temperatures  $T_f$  and  $T_s$ , you are working with two temperatures. However, you are treating that, **this you are** you are assuming that these **sorry** average temperatures of fluid and solid without incorporating local fluctuations; so **you are not** you are not considering any temperature gradient **within a** within a channel, **I mean** within

a channel where the gas is flowing or or the field, that is going through or next to that the solid material there also you will have temperature gradient.

But, you are just putting a  $T_f$  and  $T_s$ , you you do not differentiate  $T_f$  at the center of the channel and  $T_f$  at near the wall of the channel, so you do not differentiate them, so you make certain assumptions here, you do not have, so you since you do not have this, you are not considering any proper boundary condition at the wall of the channel. That the fluid, this is the fluid temperature you have this as the, that you have the solid temperature, you have the continuity of flux etcetera.

That you are not considering rather, you are clubbing everything together and you are using this  $\alpha \cdot (T_f - T_s)$  this term for the crosstalk between the fluid and the solid, so this is I mean you can you can see, this is a very mixed approach I mean you you have make you have made certain assumptions, again you are retaining  $T_f$  and  $T_s$  (Refer Slide Time: 43:00). So, one thing you must appreciate that this mean field model based on volume averaging, this gives you somewhat it should give somewhat better somewhat more accurate result than porous medium, but this is not 100 percent rigorous.

And why volume averaging look at it, how how you how you how you have considered  $\rho_f$  for example, the  $\rho_f$  the  $\rho_f$  that you used here is  $\phi_f \rho_{f0}$ ,  $\rho_s$  is equal to  $\phi_s \rho_{s0}$  and that is what you have used in this equation, you think about this equation I mean it is it is not absolutely straightforward. However, this can be this can be very useful, if you want to get some quick result, quick in a sense that you have you are given ten choices.

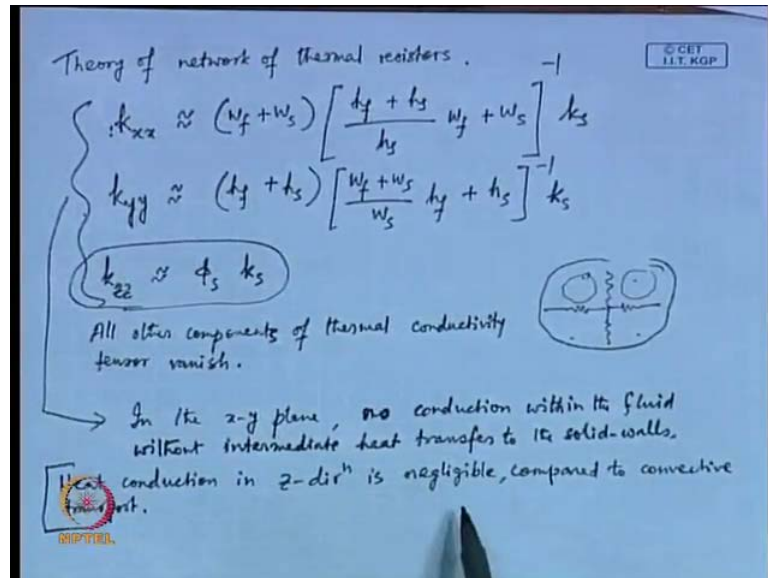
You can have  $w_s$  as this,  $w_f$  as this,  $h_f$  as this,  $h_s$  as this and you have the property  $c_f$   $c_s$  etcetera, are given and now you tell me what should be the best design of the reactor, what should be the best material for the solid part, you if you if you have to if you have to scan through it and come with the between these bounds what would be the best result you have (Refer Slide Time: 44:05).

So, if you want to do such quick calculations, then probably if you if you start from scratch and do it a detailed CFD model that may be that may require time, and it can save some time and give you some quick idea as to where you should focus on, which part you need to play with, so that you can get a better more optimum, more efficient reactor, so this is this is what we have.



Now, let me see what we have we have one one component left, we started with you remember porous medium mean field model based on volume averaging and a rigorous approach, so these these are there, now you need to understand that and and one thing I I must point out here.

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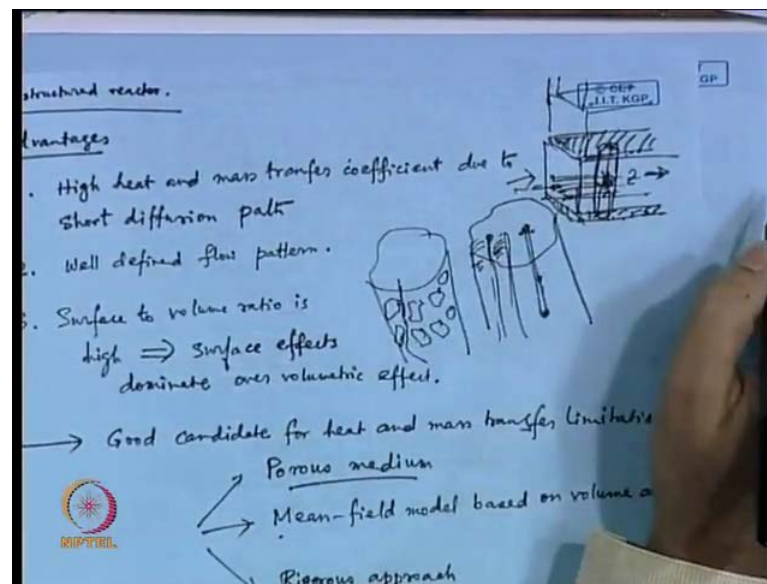
That in this mean field model, you when you when you work with this  $k_{xx}$ ,  $k_{yy}$  and  $k_{zz}$  you have you have definitely made note that in the  $x-y$  plane, what is the  $x-y$  plane whatever is the  $x-y$  plane I remember, the the way define mean field model is  $z$  is perpendicular to the paper, and the flow is happening perpendicular to the paper. So, the other plane, the cross section is  $x-y$  plane, no conduction within the fluid within the fluid without without intermediate heat transfer to the solid walls.

So, this is something which you are basically considering you (()) that you have two channels side by side, and in between you have a solid, you have two channels going side by side and you have in between flow is happening perpendicular to the paper and this is what you have, this is the block through which the flow is taking place, through which the flow is taking place.

So, conduction the heat transfer between this and this is not permitted without going through the solid part, that part you have assumed here, so that is that needs to be understood. Another thing is this heat conduction in  $z$  direction is typically negligible compared to convective transport negligible compared to convective transport this is

this is the heat conduction in z direction, z direction is in the direction of the flow, typically the heat conduction in z direction, I mean I have a  $k_z z$  term and this  $k_z z$  term is very much there,  $k_z z$  term is very much there, so heat heat conduction is possible. However, the temperature gradient in z direction that is, something which is probably causing, if this heat conduction in z direction is not very very significant, I mean if you if you look at this honeycomb.

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I mean the way this honeycomb reactor they operate, is that you have suppose you have you have a block you have block of this structure, and you have several such channels running parallel, very well defined channels you know exactly the the dimensions, and internal inner wall of these channels are coated with catalyst material. You have dipped this whole structure into the catalyst material, and you have coating of that catalyst and that is acting as a catalyst when the flow is taking place through these channels.

Now, there will be a heat of reaction may be it is it could be exothermic or endothermic, so it could be either heat would be generated or it would be taken by the reactants, so either you have to take out the heat, I mean unless the this heat of reaction is small, either you have to take out the heat from here or you have to give the heat. So, if you have one such block and then you have another block you have one such block and then you have another block here, you in between you have one layer where through which you pass the either the heating or the cooling fluid; and then you have another block on top of this and

in between you pass the heating order of cooling fluid. So, what **what** is happening here you are having a flow here, this is your z direction **right**, now you have difficulty **I mean** see, so where would be in this direction may be x or y **I mean** the transverse direction z is in the direction of the flow; so perpendicular to this, in the transverse direction you have, **I mean** what do you expect suppose here **here** there is another heating layer.

Suppose you have, you are talking about the endothermic reaction that means, the fluid is taking the heat from, so you are heating the, you have a heating layer, so you are having a hot fluid flowing through this or by some other means, you are heating this layer **alright**. So, you have this heating layer here, this heating layer here then which place would be the coldest within this block, it should be the center by symmetry, so this **this** area would be the coldest, and here it would be the most heated, here it would be the most heated (Refer Slide Time: 50:35). So, you can expect within this block there is a temperature profile.

Now, this block has thousands or millions of channels, **I mean that is** that is other issue and the fluid is flowing through this channel and they are taking the heat, **the** when the when the gas is flowing through this channel **it is** it is absorbing the heat. So, the **the** so here so, these **these** we are talking about the temperature profile in z direction and what I mentioned here is, heat conduction in z direction is negligible, what by that, **what I mean is** what is important to you at this point is that you should have proper heat conduction between this layer to here, and this layer to here.

So, that there **(())** a substantial temperature drop, suppose you are doing a, why are you getting into microstructured reactor, because you want to precisely control the temperature at which the reaction takes place, because you **you** want to avoid the side reactions. Now, this if you would have been a packed bed, **you can** you can have a similar arrangement in place, **you you** within the you can have packing and then you have heating layer around.

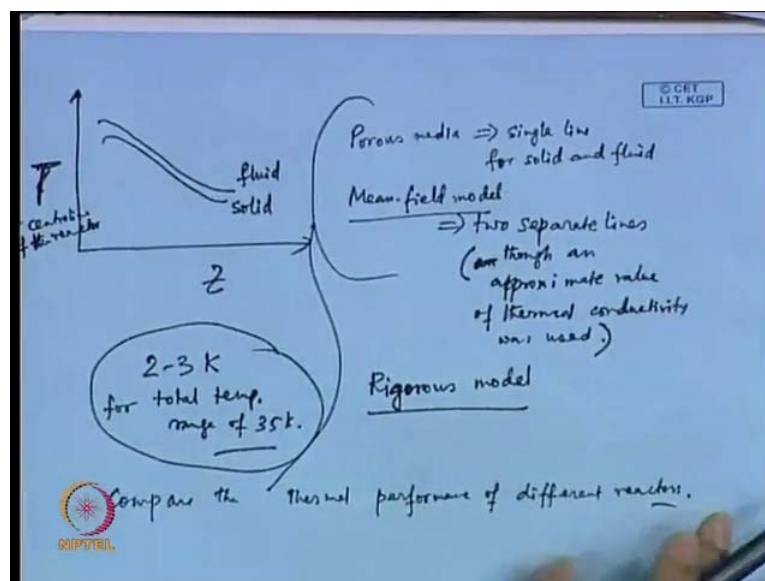
But, since it is a packed bed, since the flow this flow patterned is not well defined, what you end up with is a temperature gradient within the solid, so you would be ending up with **suppose you are** you are suppose to maintain it at say 1000 degree centigrade, and you have a gradient of say 40 degree centigrade. So, 960 degree centigrade is the temperature at which the center or the core of this is operating, so you have a gap, so you

are suppose to maintain it at say, you are maintaining the wall at 1000 may be it is that the reaction should be occurring at say 980. Now, you have that window you are creating and so you are producing side reactions, you are getting into other things, now with the reason is reason this you are choosing a microstructured reactor is that this temperature that delta t you can minimize.

When we are talking about 1000, we are talking about 1995 to 1005, that window is going to be smaller, in this in in microstructured reactor and that, so you what what we are more concerned is how this heat conduction is taking place, because this solid material that you have, should be a good conducting material. So, that you can have the flow of heat in transverse direction, now whether what heat conduction you have in z direction I mean that is that is immaterial.

Because, anyway the main main method by which the heat is transferring in z direction is by convective flow, the fluid is flowing in z direction, so that is probably what I mentioned here is as heat conduction in z direction can be, it is can be negligible. I mean I know some students who worked here, where where they have considered this z direction heat conduction as well and compared and showed to what extent it can be negligible, but it is it is the this is this is one fact which I think you understand, what I what I want mean by this statement.

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Now, we have I would like to make a quick comparison here, is that if you if you now plot temperature versus z temperature versus z, z is perpendicular to the paper that means, z is in the direction flow. So, in the direction of flow, if you now plot you will find that, you will have one is meant for the solid and other is meant for the fluid, and in case of a porous medium type model you have assumed that this fluid and solid they are of same temperature.

So, you had single line, in porous medium model you had single line at least you have two two other two different lines from this mean field approach and these are these are T at where I mean T is probably at center line of the reactor, this is a function of this. So, in case of porous medium model you will have a single line (No audio from 55:04 to 55:12) porous medium model you have a single line for solid and fluid.

For mean field model you have two separate lines however, the issue is that an approximate though an approximate value of thermal conductivity was used, so you have computational time here is saved however, the accuracy is sacrificed, if you if you if you I mean I am not going to discuss this rigorous model. But, you you know what this this by rigorous model, what we what we expect, that inside this, inside the channel you have, within the channel, within the fluid phase itself.

In a single channel there would be a temperature gradient, there would be a velocity gradient and there would be continuity in heat flux at the wall between the fluid and the solid, so if you consider those your computational time would be higher, in mean field model the computational time is saved. However, the accuracy is sacrificed and this I mean the empirical the experience is that this accuracy is of the order of 2 to 3 Kelvin for total temperature range of 35 Kelvin, that is that is some some people have found and some researcher have found showed, that you if you if you if you do this you sacrifice the accuracy.

But, this sacrifices of the accuracy is also can be quantified and this is not a very large quantity, I mean at least you can you can do the screening of the materials, screening of various geometry using this method and finally get the final result using a detailed CFD model. And these, so you can compare the thermal performance using these mean field and the porous medium model, you can compare the thermal performance of different reactors and because, compare the performance you need to run it

several times and probably, that you would be the computational time would be a concern, if you use a rigorous model.

So, I think you understood what, I mean the how some approximations can be done, where you and and still you can get some result, some approximate result for this microstructured reactor. And in the next class, we will be discussing about theas I saidimmiscible flow through microchannels,we will start withthe first the definition of Laplace pressure, and then we go from there, that is all I have for today's class,thank you very much.