

**Multiphase Flows**  
**Dr. Rajesh Kumar Upadhyay**  
**Department of Chemical Engineering**  
**Indian Institute of Technology, Guwahati**

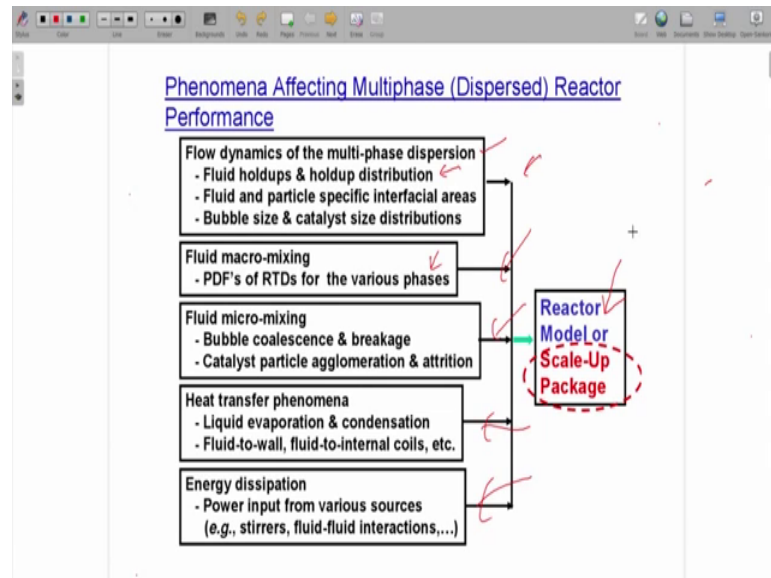
**Lecture - 14**  
**Introduction to Multiphase Flow Modeling**

Welcome back. So, today we are now going to restart the next phase and in the next slot whatever we are going to discuss is about the modeling of multi phase flow reactors. We have already discussed some of those modeling parts during the previous phase and during the discussion of the pressure drop and once we have written the equation for into a 1 dimensional domain. Now what we are going to do? We are going to see the 3 dimensional modeling.

So, till now whatever we were discussing; we are discussing the equation and most of the thing our discussion we have limited ourselves in the 1 dimensional domain. Now we will move towards the 3 dimensional domain and we will see that in the 3 dimensional domain, how the equation will be modified? And how to solve those problems, for second thing we were not talking about too much interactions till now.

Now, we will see that different type of coupling and different interactions and how to incorporate those interactions so, that we can do the simulation or modeling or the industrial scale equipment. So, to begin with what I will do I will search revise some of the fundamental so, that you again actually come to the same label and we understand that what is he need in the modeling. And why we do the modeling of any multi phase flow reactor or any modeling at all.

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So, whatever we have discussed till now, the phenomena which affect the multi phase flow reactor performance where there is a discrete or it is a continuous dispersed phase or it is a continuous phase is actually the flow dynamics of the multi phase dispersion. So, how the flow dynamics is being involved that is what its effects and once we say the flow dynamics; what we mean is that the fluid holdup the holdup distribution, it means what is the holdup or phase fraction or volume fraction of a particular species or particular phase and how it has been distributed.

Then we mean about the fluid and particle surface or interfacial areas that how they are; what is their surface area what is the interfacial area in between them the size of the bubble catalyst size distribution and all those particle size distribution which we have discussed that how they are changing. Then how the mixing is taking place now mixing can be get from the RTD ok. So, how this mixing is being taken place or will take place then we want to understand that how the bubbles; if suppose there is a bubble column and then what happens we said that as a single bubble which is moving up.

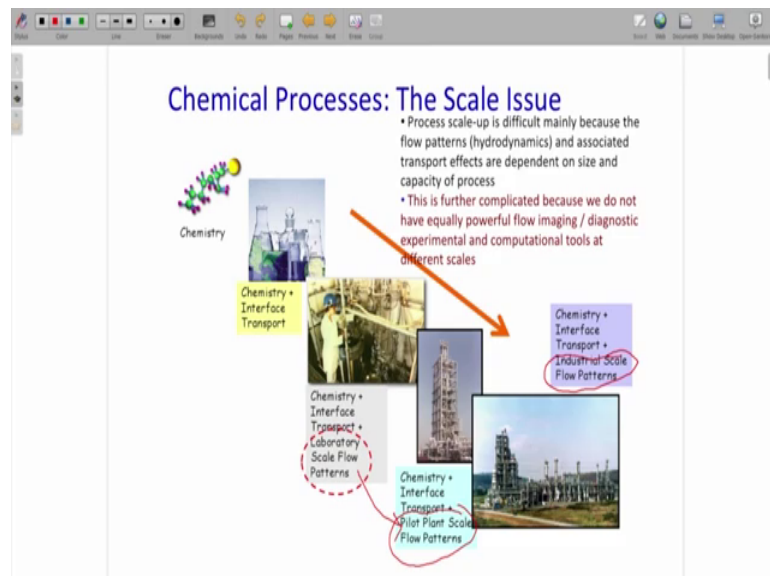
Now, we can talk about that how the multiple bubbles are moving up, how they are coalescence or breaking or taking place, how the catalyst particles are moving together we will have some attrition and agglomeration; we need the information for that. We need the information from the heat transfer phenomena like liquid evaporation

condensation of fluid to wall these interactions and all; we need to find that and then how the energy is being dissipated ok.

Now, this energy dissipation can take place from the various sources like if you put a stirrer that will be there; the fluid fluid interactions the viscous forces all those things will actually add to the energy dissipation. So, this is what we want to understand and that combined package is called reactor model ok. And this reactor model is actually very critical, particularly once we are thinking about this scale of methodology. So, that is the main motivation of doing any reactor model so, that we are performing the experiments or we are understanding the system at one scale we are doing the modeling we are rigorously validating our model at that scale.

And if I have done everything correct if I have incorporated all these variables whatever we have discussed properly, then we will have a reactor model and that reactor model can be used effectively to predict the performance of the reactor or behavior of the reactor for different operating parameters. And the same reactor model can be used to is for the scale of studies or for the scale up of the reactor. So, that is the whole region that why we go for the modeling and what is the need of the model.

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Now, as I said earlier that how the whole chemical process has been developed. So, we start with the basic chemistry and that basic chemistry we develop at the flask scale. Then we move to the laboratory scale system now in the laboratory scale system what we

do we introduce the laboratory scale flow pattern then once we move from laboratory scale system to its success we move the laboratory scale system to pilot plant scale system, what will happen? This laboratory scale flow pattern will transform to the pilot plant scale flow pattern rest of the chemistry and interface transport remains same.

If we get success further we further move to the industrial scale system and what happens? This pilot plant a scale flow pattern is actually changed to industrial scale flow pattern and in chemistry and interface transport remains almost same. So, this flow patterns actually keep on changing and we need to predict that flow pattern and why it is still a challenge whatever we have discussed till now; is the reason is that neither we have a measurement technique which can measure the flow performance or performance of the reactor with equal accuracy at all the level. So, that is the one major kind of a problem.

Further even to adding into that forget about that the accuracy remains same at all the scale, none of the technique is available till now experimental measurement technique which can give you all the parameters required for the scale up even at a laboratory scale. So, we need to build upon the experimental technique similarly the models which we are going to discuss or whatever we have discussed earlier also in 1 dimensional I have keep on telling that each model has certain limitation. So, that is true with the modeling part also that we do not have even a computational model available or numerical model available which is equally valid at all the scales.

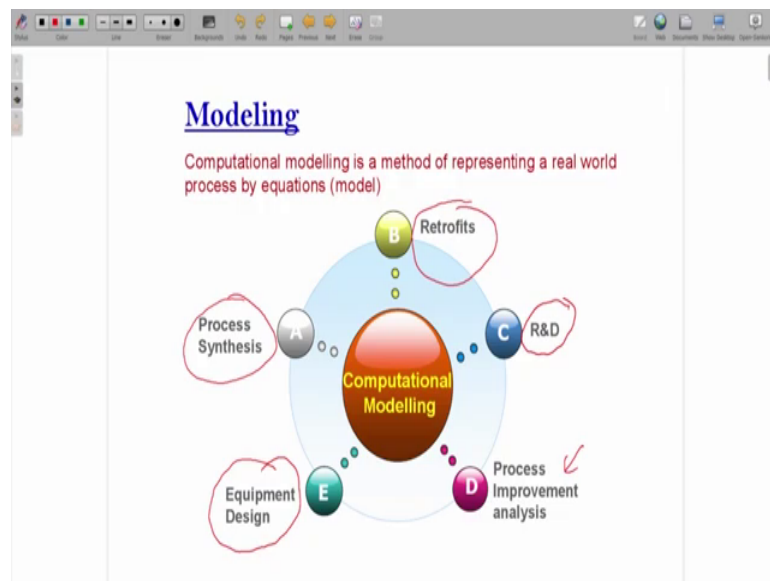
And that is the problem in this scale of strategies that why we are not able to do this scale up properly which is completely based on the science. So, to resolve that we need to understand the limitation in the measurement techniques, the limitation in the modeling technique or numerical techniques and we should use the appropriate model depending upon the requirement. And then we should based on that model we should scale up the reactor or predict the performance of the reactor and we should know that what is the limitation that is very critical to understand that whatever the model I am using.

What is the limitation of that model, how far this model is valid, how much accurate the model can predict the flow phenomena or predict the physics? So, that is what is the aim of this section and we will try to see the different modeling approach; some of them we have already discussed now in do some 3 dimensional modeling do some rigorous

interactions also and how to solve the equations, for the different ranges or different domain and we will try to discuss their advantage and disadvantage and limitation.

So, that is the whole thing which we are going to discuss and we will be mainly focusing in this section not on the experimental technique, but we will be mostly focusing on the numerical simulation.

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So, what is modeling? So, computation modeling is nothing, but to is a method to represent a real world process by equation ok. So, that is what is modeling is; so, you see any phenomena like if I am moving you are seeing my movement and if you write that movement in terms of the equation that is called modeling ok. So, modeling is nothing, but writing any physical phenomena in terms of the equation and why we do the computational modeling; because it helps us to analyze the physics.

It helps us to understand the flow or understand the physics and it can kind of prevent or it can kind of minimize the experimental measurements; so, you do not need to do the measurements all the time ok. So, if you have a fitted model suppose if you are able to model my movement; you have to just do the measurements, once you have to fit an equation on the my movement which will be model equation which will predict my movement by behavior and next time you do not need to do the modeling again; you can keep on predicting the motion my motion all the time ok. So, that is the main reason that

why we do the modeling and main aim of the modeling, you can say has can be divided in these parts.

The first aim is definitely the process synthesis that a model can help me in the synthesis of the prop this process. Now that model will be actually based on the molecular model we can have a DFT simulation, we have a molecular simulation to see that how the two species will react each other. So, instead of performing the reaction we can do some modeling, we can say that whether say if I take a species A and species B whether they are going to react or not.

So, instead of doing the experiment wasting money on the experiments; I can do the modeling I can even predict a priori that these are going to be react and what will be the possible product or possible product distribution which will come out of these two reaction or when the species a and species b with reactive to each other.

So, it helps me a lot to analyze the process to analyze the process synthesis that how the process would take place. Then it also help us in retrofits it means what it helps us in troubleshooting, if you have a some problem you want to redesign, you want to improve that design, you want to correct some mistakes whatever is being done either in the design or in the process conditions; you can do it with the retrofits because we already have a model available I can understand that this model will be sensitive to this parameter or if I change the design it in this way; how my model performance is going to change and how not model performance, but how my reactor performance is going to be changed.

So, if I have a model available I do not need to do the experiments for all the troubleshooting what I can do if my model is well, if its predicting well I can do the retrofits. So, that is the typical use of the model and very very critical use of the model to in the retrofits. So, that we can do the improve troubleshooting we can improve the existing equipment design and all and even we can find the optimal parameters for which the reactor or the process vessel should be operated.

Then R and D is a very very critical part; we know that R and D is pretty much money governed and you have to spend a lot of money if you have to do the experiments for all the possible conditions, it will be very very expensive. So, if you do the model fitting; you can minimize the cost of experiments, you can understand the physics and that is

very very critical because if I can write any process in terms of the equation; only if I understand the physics of the process ok.

So, if I understand the physics of the process definitely my predictions will be much better and I will also save on the money wise. So, I do not need to spend the money for all the experiments; I can I do not need to do the experiments for all the possible conditions, all the possible sets; all the possible internals and all. So, I can do the experiments for certain sets, I can develop a computational model and that computational model will help me to understand the physics of the reactor. And then I can analyze the performance of the reactor in presence of many other things.

So, I can do it for one case and then the other cases like without internal, with internal, for different velocity conditions, for different pressure conditions my model can give me that how the performance of the reactor or process vessel is going to change. Then it can also help in improving the process as I said that the process you can analyze the process you can understand the physics of the process. So, you can analyze the process and can improve the process that if suppose some processes some say CSTR is there where they is impeller which is rotating inside you are finding that your model is predicting that the mixing quality is not very good.

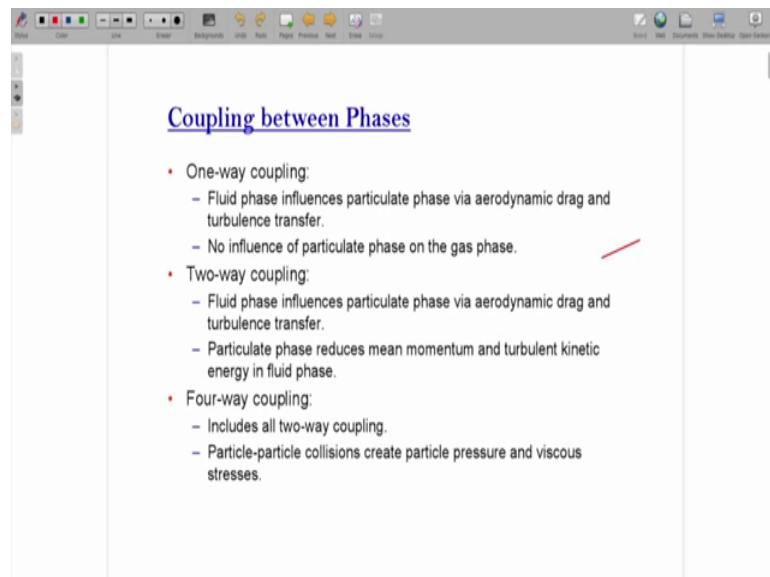
The diameter of the CSTR vessel is very high compared to the impeller diameter. So, to improve the mixing we can think about putting the baffles on the wall. And we can do our modeling with the model equation and we can see the effect that whether if I put the baffles and whether it is going to affect positively in mixing wise or not. So, all those process improvements; so, I can put the if it is improving I can install the baffles. So, I do I have not done any experiments well just with the modeling I can do this job. So, that is another very very critical thing to improve the process performance we can use the modeling and definitely the equipment design and scale up is one of the critical parameter that why we do the modeling.

If you see that most of the equipment is being designed based on the model equation, those model equation which we develop based on the experimental data or we fit the model equation and then we validate those model predictions with the experimental data that model is being widely used for the equipment design. So, like for heat exchanger we did the experiments for your times, we fit some model equations and that model

equations are being used now even till now to design the heat exchanger. It is not like every time to design the heat exchanger you need to go and perform; make a setup, perform the experiment, measure the delta T, measure the flow rate, measure the pressure drop; you do not need to do all those things.

Just with the model equation which has been developed; then you can do the heat exchanger designing. So, these are the major advantage that why we want to do the computational modeling, why you want to have a 3 dimensional model to understand the flow physics.

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So, what we have done till now we have discussed about the interactions, but most of the interactions was actually we discussed in the one way coupling or one way interactions. Like fluid motion is affecting the particle motion or particle motion is affecting the fluid motion and we have developed the one dimensional equation based on that; the rigorous interaction part we have neglected.

But once we are going for the computational modeling or rigorous modeling, we cannot remove or we cannot neglect the interactions which are taking place between the different phases. Why? Because these interactions are the one who is going to govern the flow physics inside the vessel of interest. So, it is very important to have different interaction and to have that interaction in the model equation, you should understand that what kind of a coupling take place between the different phases ok. So, there are mainly

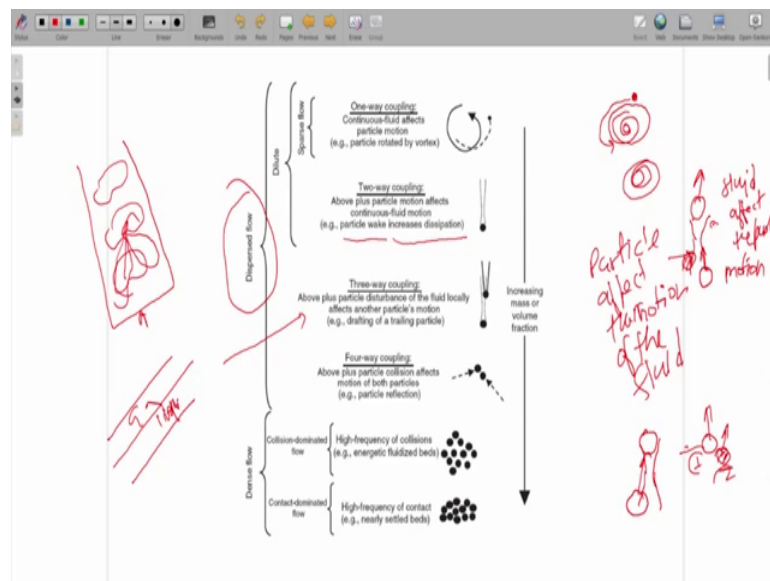


four type of coupling or four way of coupling; we call it one way coupling, two way coupling, three way coupling and four way coupling.

Now, what is one way coupling and all? So, one way coupling means the fluid motion is actually affecting the particle motion and particle motion is not affecting the fluid motion that is called one way coupling. Similarly in two way motion of fluid is affecting the motion of particle, motion of particle is affecting the motion of the fluid. So, you have to have a two way coupling.

Now, if you are having a two way coupling what you need to do? You have to include the drag in both the equation or both the phases. Similarly we have three way coupling and four way coupling. So, to explain that let us I will move to the next slide.

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And this is the slide where we can explain that what does the one way coupling, two way coupling, three way coupling and four way coupling means for.

So, as I discussed that for generally gas solid flow or any flow any multi phase flow we can divide in two parts; one is called dilute flow and one is called dense flow ok. Now we can divide it as a dispersed waste flow and dense flow and dispersed they flow can further be divided as a dilute flow. So, what do you mean by the dilute flow? When the particle fractions are very very small or discrete particle fraction is very very small; the

flow is called dilute flow where the stokes number is also less than 1; so, that is called dilute flow.

If stokes number is more than 1, your particle fraction is very high then what will happen? The flow will be actually the dense flow we have already defined that the dilute flow and dense low definition you can just see that the stokes number is not the real place; we have already proved that when the flow will be dilute when the flow will be turbulent; whatever stokes number I said is actually just a thumb rule.

But there is a formula where we can use that and we have already derived that formula from the dilute flow and dense slow conditions. So, in the dilute phase flow roughly speaking the particle fraction is very low less than 5 to 10 percent; you can say that the flow is dilute and in that case we generally use either the one way coupling or two way coupling. Now one way coupling means what? The fluid motion or continuous phase motion is affecting the motion of the particle ok; so, that is called one way coupling right.

If suppose you have a particle rotation or particle rotated by the vortex. So, suppose if you go to river you see some vortex formation or A D formation; now that vortex formation suppose this is the vortex formation which is taking place. So, if there is any particle in this domain what will happen? The particle will also start moving it in this thing once the particle will go too near to the vortex which will also start moving it in this way. And it means what? The fluid motion is actually affecting the motion of the particle and that is called one way coupling.

The particle have no say in that there is only single particle which has been stuck in the vortex then what will happen? The particle will start moving with fluid and that is means the fluid motion particle motion has been started only because the fluid motion was there. So, it means only the fluid which is affecting the motion of the particle. So, in that way the equation we solve we call one way coupling ok.

So, what we do? We see the motion of the particle, how the motion of the particle will be taking place? We will in fact, will add one way coupling and that one way coupling in this case is mostly from the drag. So, we use the drag equation; we saw the drag for the particle motion to see that how the particle motion is being affected with the fluid motion or in fluid motion we do not include the drag factor then it comes to two way coupling.

So, two way coupling is approximately same whatever it is there, but a solid motion is being affected by the fluid motion and fluid motion is affected by the solid motion ok. So, that is why it is called two way coupling; so now, our earlier what we said that there is A D formation a particle comes within the AD; it is start moving with the AD or with the vortex and the vortex flow or vortex motion is not being affected at all; while the particle motion is being affected and particles start moving in the vortex wave. So, it is start circulating; so, that is the one way coupling, in two way coupling fluid motion is going to affect the motion of the particle; particle motion is going to affect the motion of the fluid ok.

So, the best example for this is the wake formation behind the bubbles or the particle. So, suppose a particle is moving and its moving because of the gas velocity a gas is being passed; there will be a wake formation behind the particle and that you will see like something like this. And because of this wake formation what will happen? The fluid motion will also get affected. So, this is called two way coupling; so, particle motion is affecting the motion of the fluid, the fluid motion is affecting the motion of the particle ok. So, that is two way coupling and it generally take place in the particle wake whether the increasing dissipation is there.

So, where the particle wake is there, where the energy dissipation is very very high or it is keep on increasing; this two way coupling is very very critical ok. So, that is for the one way and two way coupling both the coupling does critical for the dilute phase. So, once you have a dilute phase, you can have one way coupling or two way coupling. Generally one way coupling and two way coupling is both is being governed by the drag force itself.

So, in one way coupling; we solve the drag force in one phase in two way coupling you solve the drag force for both the phases ok. So, that is the difference in the model equation and both are valid for the dilute phase flow. So, if you have a dilute flow you can use only either one way coupling or two way coupling; depending upon your situation. Then comes the three way coupling and three way coupling says what? That whatever we have discussed that the fluid motion affect the motion of the particle.

Particle motion affect the motion of the fluid, we also find that the fluid locally affect the another particle motion ok. So, it means what? Fluid is affecting the motion of the

particle; particle is affecting the motion of the fluid and fluid motion is not affecting the motion of one particle, but it is also affecting the motion of the other particles too. So, like if I take this case ok; so, the gas was passing up particle is start moving with a high velocity it will form a wake ok. So, what happens the once the wake has been formed was the particle a once the particles start moving it means particle effect fluid effect the particle motion motion.

Then because of the particle motion, wake formation take place this wake formation says that particle affect motion of the motion of the fluid. Now because of this wake formation, if suppose there is another particle which is somewhere here what will happen because of this wake formation the particle motion will further increase and; that means, the particle motion fluid affect the motion of the particle; particle effect the motion of the fluid and then the fluid again affect the motion of the other particles which is not affecting the only one particle; it is affecting the motion of this particle of this particle too whichever is comes in the region of the wave.

So, that is called three way coupling ok. So, that is called three way coupling; three way coupling is being used when the solid fractions keep on increasing or the particle dispersed fractions keep on increasing; three way coupling becomes important because you have a wake formation and in the wake the particle comes in. And we have already discussed a lift force during the discussion of the lift force; suppose there is a bubble column where one gas bubble is being injected inside and that gas bubble is actually moving. And because it is gas bubble and the shape of the gas bubble is generally in the mushroom shape you can say that something of this kind of a wake formation will take place.

Any bubble which will come in this range will actually go and have a coalescence with the previous bubble because this velocity will keep on increasing. And because of that these two bubble will have a coalescence and they will form maybe a bigger bubble what they may break into the two smaller bubble. So, in that cases where the wake formation is being taken place; it is very evident we use the three way coupling ok. So, four way coupling then the next coming to the four way coupling.

Four way coupling means all three above whatever we have, we just say that the particle is also affecting the motion of the other particle. It means what? Fluid is affecting the

motion of particle; particle is affecting motion of the fluid fluid is affecting the motion of the other particles and particles are affecting the motion of each other. So, that is called four way coupling; now we have all the four way coupling, the four way coupling the fourth coupling is mainly because of the particle collision.

So, suppose again the same example if I have this for particle which is moving up in the air or in the because of the air and form a wake formally. And then you have a second particle which is actually been there and that is actually motion is get affected because of this wake formation and they goes and heat each other ok. So, they goes and hit each other; so, like this.

So, what will happen now? This because of this interaction or because of this collision the particle which was saying earlier moving straight may start moving it in this direction ok. So, what will happen? The first particle movement it means say this is first, this is second the first particle movement has changed because of the collision of the previous particle or next particle which has been taken place. So, what it will be? It will going to affect the motion of the solids.

So, what we are going to model is that that the fluid is affecting the motion of the solid; solid is affecting motion of the fluid; the fluid is affecting motion of the other solid too and solid is affecting the motion of the solid. So, that is called four way coupling all the four way coupling; in the dense phase what we say that this is sometimes dominating based on the collision dominating. It means what? So, first four whatever we have discussed is actually present everywhere.

But for the sake of simplicity in dilute phase flow we know that the particles fractions are very very small; they are very far from each other. So, the phenomenon are kind of the three way coupling and four way coupling; if it is there it will be very very low compared to one way coupling or two way coupling. So, that is the reason that for the dilute fluid slope; we remove the three way coupling and four way coupling and we just consider one way coupling or two way coupling depending upon the application.

Well if you keep on increasing the solid fraction; you cannot neglect the collision, you cannot neglect that the fluid performance of fluid velocity is going to change the performance or the velocity or the characteristics of the next particle. So, that is the reason that we introduce the third wake or three way coupling and when if it is further

improved or further increases the fracture the discrete phase in the flute; you can say that now the four way coupling will be required because everything is going to affect the motion of each other.

So, that is the way the four way coupling is being done; in most of the cases that is why we write it at your disposal why because these couplings are important, only if both the phases are one phase is at least dispersed. If both the phases are continuous then some disk couplings are not that much relevant because they are not going to affect the motion of each other. So, they will affect, but not it in the great way say stratified flow where gas is on the top liquid is on the bottom ok.

So, what is going to happen? If you do that you are going to see that phase, then what will happen that because this is a continuous phase; you are not going to change the things in the that great way. So, what will happen that because the flow is continuous the interactions will take place only at the interface. So, they will affect, but they will affect only at the interface and because there is only a clear cut interface; it is not possible that the motion of gas or motion of the fluid is going to affect the motion of the other phase other particles because only at the interface the flu can be come into contact with each other.

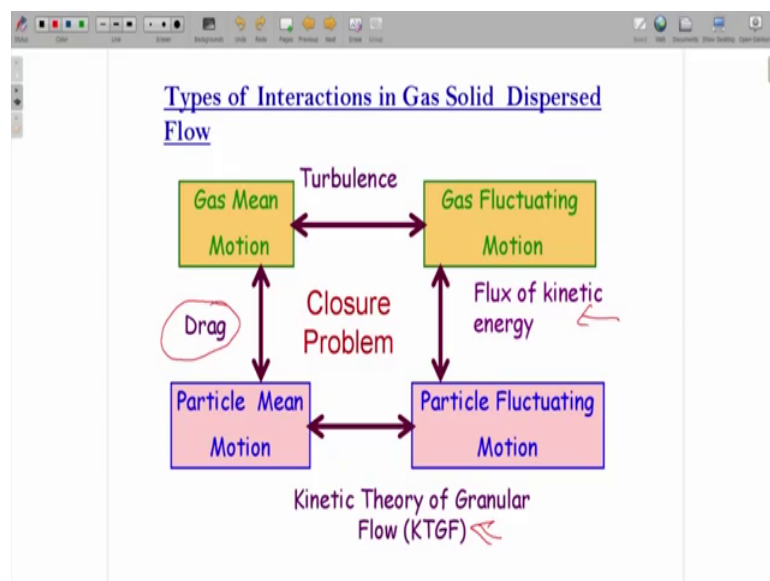
So, that is why all the four way coupling happens only if one the phase one of the phases in the dispersed phase condition ok. For dilute phase one way coupling or two way coupling is acting, for a very highly concentrated flow like a fluidized bed kind of a flow the flow actually has been found to be collisional dominating ok. So, that is the kind means that fluid is definitely going to affect the motion of the particle; particle is going to affect the motion of the fluid.

But the major problem is the collision between the particles is actually going to govern the physics of the bed. And that is the case once the volume fraction of the solid or discrete phase is very very high like in the fluidized bed which is just started fluidization or you can say the fluidized bed operated at a minimum fluidization velocity or just above the minimum fluidization velocity; the flow actually will be pretty much collisional dominating because there is not much movement of the solid they started vibrating.

But the bed expansion is very low. So, whenever they try to move actually the particles try to move it with other particle and then changes the direction; changes the motion; so, it is called a collisional dominating flow. Similarly they are certain flows like settling where the flow is contact dominating ok. So, it means what? The particles are being said how they are contacting with each other; they that is going to affect the motion. So, that is called contact dominating flow; the one where the fluidized bed is there which is being operated just above the minimum fluidization velocity, the flow is affected because of the collision. So, that is called collision or dominating flow.

So, these are different coupling is there and based on the application as I said; we introduce the coupling, different type of coupling in our model equation. So, this will be very sure that what we are introducing, what is the purpose of this and why we are doing all this? So, that can be understood with this coupling equation or this coupling thing.

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Now, as the coupling is done; we need to solve the equations and as I have already discussed that those equations are actually not complete; it means number of variable is more compared to the number of independent equation you are already having. So, what you need to do? You need to use some additional equation to solve the process also solve your compositional model. So, that can be done by using the closure problem.

So, what we have we have already discussed that this slide also we have discussed I am again introducing it. So, that we can understand very clearly that in the model equation

when we are using the other terms and what is the role of the terms? So, as we said earlier also that the gas mean motion or fluid mean motion is actually correlated with the fluid fluctuating motion and that correlation is being modeled by using the different turbulent models.

Now, you are free to use the unique turbulence model whatever you feel like or whatever it is applicable. Now I am not going in detailed of that what is the turbulence models and different type of Cardenas model; what is the limitation of each turbulent model and applicability of each turbulent model. So, let us assume that you understand about the turbulence model. So, depending upon the condition you can use a suitable turbulent model to model the interaction between the gas mean motion and gas fluctuating motion.

And then it comes the interaction between the different phases. So, that interaction actually the interaction between the different phases like the gas mean motion of the fluid mean motion is going to affect the particle mean motion or disperse phase mean motion. And that has been modeled by using a drag equation which we have already discussed. So, depending upon the condition again fluid we can use Sila Norman module immoral agenda if it is a fluid and solid then we can use carrasco when and you all these correlations ok.

So, based on the condition the mean velocity of the gas and mean velocity of the particles are being actually related or can be correlated by using the drag. Then because the particle is also moving or dispersed stage is also moving, what is going to happen? If it is a solid the dispersed phase mean motion of particle mean motion is going to be get affected by the particle fluctuating motion. And that the correlation between this or can be model by using the kinetic theory of the gases.

We will discuss what is kinetic theory of gases; so, the mean motion between mean and fluctuating motion of the particles can be modeled by using KTGF or Kinetic Theory of Granular Forces and the gas fluctuating velocity can be interact with the particle fluctuating velocity and that interaction can be modeled by the energy of kinetic flux ok. So, these are the different closure equations are available and together with they actually close your equation.

So, these are the different closure equations is available which you have take care while modeling any process. So, what you need to do in the morning again I am telling you that



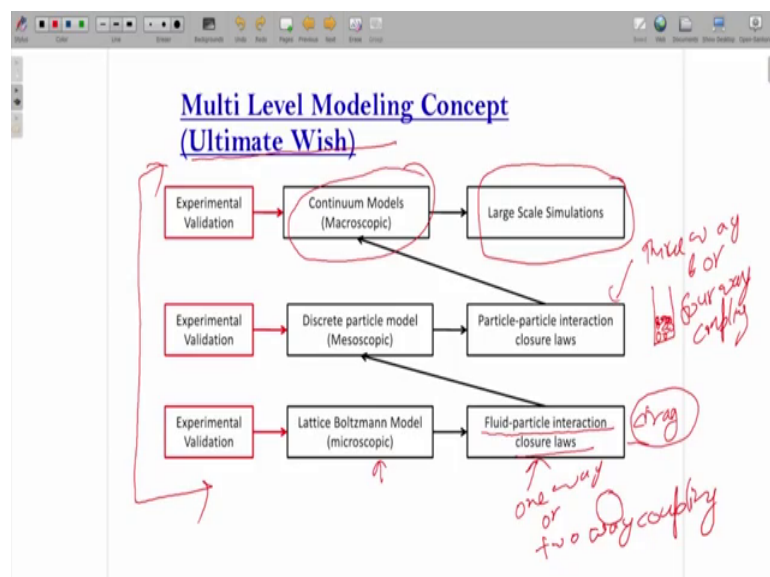
what you need to do; you need to understand the process first for that what you need to do you can reduce kind of you can find that depending upon my process or depending upon my operating condition; what kind of a coupling I should incorporate, whether it should be one way coupling; whether it should be two way coupling whether it should be three way accompanying or four way coupling.

Now, one can argue why I need to think this much I can use all four way coupling all the time. The problem is if you are using four way coupling, you are solving the equations more equations solving more equation is computationally expensive as well as it will require huge time without getting any additional benefits. So, if you do not say a very dilute flow through a flow say particle fraction is less than 1 percent.

If you use collisional equation also if you use that your three way coupling also your collisional equation or four way coupling also your two way coupling also what will happen you are increasing the number of equations which you need to solve simultaneously. So, you are increasing your computational time and the computational requirement.

So, that is the reason we should understand that what are the forces which are critical, what are the closure equations which are critical and how to use that closure equation so, that I can predict the motion of the particle or I can predict the behavior of the reactor with much accuracy ok? So, that is the reason why we understand to understand all this.

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So, now what should be the approach with you understand the system what should be our approach modeling approach? We call it multi level modeling concept and that is the ultimate wish that is why I said that ultimate wish is one day will come then I will not dependent on the experimental data at all; I will be doing everything so, the model development. Like if I have to make a process; what I will do I will first do the molecular simulation or DFT calculation to find that whether the experiment within the species A and species B will take place or not.

Once I have been able to do that what I will do? I will take that equation; I will do the molecular level simulation that by using the lattice Boltzmann equation; that will be across one particle scale. So, what I did? First I did kind of a simulation or molecular dynamic simulation try to find it out its suppose I have to react a species A and this is B under what condition the reaction will take place whether I need the solid catalyst or not and also once I have synthesized the process, I know my process requirement.

Once suppose my process requirement says that I have to use discrete phase reactor or it is a gas solid reactor, then what I will do? I will first do the lattice Boltzmann simulation though I am not going to discuss the lattice Boltzmann simulation in this course the different is scope all together; you can read about it if you are interested. So, what I am going to do? I am going to solve the lattice Boltzmann equation to find the particle and fluid interaction and that I will do across one particle or few particles ok.

So, once I will develop that equation what this equation will give me? If this equation will give me a closure equation which will interact with in the fluid and particle interactions and that is nothing, but the drag. So, I will get the drag equation from this place that how much drag will act and how the drag equation should be there look like for this condition.

Now, once I have a drag equation there; we will solve a discrete phase model equation we will discuss what is discrete phase model equation; it is an island Lagrangian approach that is called a media scopic scale. So, first one was the microscopic because we are doing across one particle a few part one or two particles or few particles. Then we moved to the media scopic bed; it means they are doing at a bed scale, but that bed scale is very very small.

So, say we are making a reactor with a very very small size say 10 centimeter or sorry 10 mm or 2 centimeter or 3 centimeter in diameter a very say 10, 20 meter in the bed height and we do the simulation here we write the discrete phase model equation and we try to find it out the particle interaction phenomena. So, in this way I have developed the correlation for one way or two way coupling.

Now, this will actually give me three way and four way coupling and or four way coupling, it will tell that whether the three way coupling or four way coupling is important or not and what should be the correlation for that? And then we used in the continuum model and the continuum model as the name suggests you are going to solve the Navier Stokes equation again I will discuss the equation. So, do not worry about that, but the continuum model we will use and we will now do the validation at the large scale.

So, why we are doing it? Lattice Boltzmann equations are computationally very very expensive. So, that is why we are solving only across one particle; beam simulation or dp and simulations are again computationally expensive, but not as of Lattice Boltzmann equation. So, we have increased our scale at a certain scale we are trying to solve that interactions and we are getting the interactions. And then we are moving towards the continuum model where we are using all the equations or interaction closures which has been developed with these approach.

And then they are solving at a large scale for the scalar for large scale reactors ok. So, that is the ultimate wish now why that is a wish? Because right now we cannot do any of these simulations without having the experimental validation because our numerical approach is not being matured enough, they still have lot of assumptions to solve those equations and because of that you because you are using those assumptions; you need to validate your assumptions and that is why the experimental validation is required. So, this is a dream if I am working in the multi phase flow, I always want to have a dream or I always have a dream that I will do everything based on the model I do not need to do the experiments.

But right now the state of the art is not of that kind and that is why the experimental approach is needed. And these links are not still well established that how to use those equations in the other scale ok. So, that is what is our wish ultimate wish and we will

come to this slide that what is the different types of multi phase flow models approaches there and how difficult or how easy they are we will discuss it, but that this is not the time I think I will discuss it later on after discussing this.

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		Gas liquid flows	Gas solids flow		
M O R E  P H Y S I C S		VOF	Lattice Boltzman	M O D E L I N G	
		interphase tracking			
		Bubble tracking	DPM		
		Multifluid	Multifluid		
			Multifluid and bubble tracking		

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**Modeling Approach**

- Empirical correlations
- Lagrangian Track
  - Track individual point particle
  - Particles do not interact
- Algebraic slip model
  - Dispersed phase in a continuous phase.
  - Solve one momentum equation for the mixture.
- Two-fluids theory (multi-fluids)
  - Eulerian models.
  - Solve as many momentum equations as there are phases.
- Discrete element method
  - Solve the trajectories of individual objects and their collisions, inside a continuous phase.
- Fully resolved and coupled

*Handwritten notes:* "Euler - Euler model" (circled), "Increased complexity" (vertical text next to a blue arrow), "30% Solid 70% Gas" (circled), "More Physics", "more expensive", "more complex" (written vertically on the left).

So, what we are going to do? The approach is to write the phenomena in terms of the model equation and as we have already done there are different type of model equations are available. And depending upon the process conditions the approach, we are using the accuracy required the understanding required we use different type of modeling approach

and depending upon the coupling also. So, they are different modeling approach and what is that different modeling approach is actually; first is the empirical correlations that is also a model, you perform the experiments based on takes you up the data random generate the data.

Based on the data analysis you fit some equation and that is called empirically fitted equation and empirical correlations and you use that correlation to predict the phenomenon. And that are widely used this kind of a correlation for the single phase flow. Remember any of your single phase flow reactor design like heat exchanger or any other single phase flow reactor design; this all are based on the empirical correlations which has been developed by performing the experiments, we deprived the equation, we develop some correlation and we use that. So, that is also a modeling approach ok.

Differently that empirical correlation even in multi phase flow are widely used like Lockhart Martinelli correlation which we have discussed, but there is a serious limitation of those empirical correlation they are at least only valid for a particular range of the condition for which the experiments has been performed ok. So, that has been limited and the accuracy is being seriously limited to that range and we have discussed that while discussing the Lockhart Martinelli correlation that it is just being used to get the firsthand idea.

Then we can use the Lagrangian track the equations which we have solved in one dimensional domain; we are tracking the particle one particle we are tracking just individual particles of one particles only. And we do not assume that the other particles are affecting the motion of each other. So, what we have done till now? In the in this in the Lagrangian track, we can use that to find that we can use that approach to model the reactor performance, but the only thing is you can include only one way coupling or max to max way coupling.

Generally the include only one way coupling the way we have solved that there is a fluid the particle is there in the fluid and the particle motion is get affected because of the fluid we solve the fluid motion particle motion by solving the Newton's second law of motion we use that the forces and the drag force becomes a very very critical. So, you can use that Lagrangian track approach, but there is no way you can include the three way

coupling two way coupling you can still think about you can start solving the gas wedge equations simultaneously both the equation and keep on updating.

But we do not solve particle interactions in that case; so that is why it is called Lagrangian track it is relatively simpler. Then we go to algebraic slip model and here on what we have discussed these two we have already discussed not the empirical correlation we have discussed only for one case in the multi phase flow Lockhart Martinelli; there are several empirical correlations are there, we are not going to discuss that Lagrangian track we have already discussed till now.

Now, what we are going to discuss is the rest of the thing. So, the another set of the thing is algebra slip model; in that algebra slip model as it says that it based on the slip velocity or drift velocity we will discussed this. This has been used for the dispersed phase in a continuous phase, it means one phase should be dispersed another phase should be continuous then we use the algebraic slip model.

And in this what we do we solve the equation for one equation, one momentum equation, one continuity equation based on the mixture property ok. So, it is very similar to the homogeneous model which we have developed earlier we were discussed earlier in the 1 direction, 1 dimensional domain; we will discuss it further here algebra slip model which is very similar to that and we will discuss that how the equation will be modified in the 3 dimensional domain.

So, what we are going to do? We are going to solve one continuity one momentum equation and both the continuity and momentum equation will be based on the mixture model mixture properties. And we will also solve the volume fraction equation we will see that recurrence we will discuss the equation we will see that volume fraction equation will additionally solve which is different from the homogeneous model. We will see that how the fraction though this phase is changing with the time and with the location.

So, these three equations will be solved together to find the reactor behavior or vessel behavior. Then it is called two fluid model or popularly known as Euler-Euler model Euler-Euler model this is widely used model and it is the model which you can use I will say that this is a single model otherwise the Lagrangian track even that is difficult to implement at industrial scale.

The simple single model as of now which we can kind of implement at an industrial scale system with a reasonable accuracy; I am putting single model because I quoted reasonable accuracy you can use algebraic model also, but the accuracy will be limiting and the approach will be also limiting for a particular condition, but the two fluid model is widely used and ideally you can use it for most of the conditions. And you can use this for all these scales whatever the scales we understand even at the industrial scale even with the current computational power you can use that.

So, what does it phase says that this is the Euler-Euler approach now what is Euler-Euler approach? In Euler-Euler approach we assume that both the phases which are present or all the phases which are present in the reactor or in the process vessels are continuum. It means they are a continuous fluid and interpenetrating fluid. So, they are actually under interpenetrating continuum.

Now, what do you mean by interpenetrating continuum? So, let us try to understand that suppose I have a bed and I will explain it for more clarity as a gas solid say this is gas phase which is being injected from the bottom there are some solids are present. Now what will happen? If I take a small domain and I see that where the solids are present, where the gas are present, I will say that this is the place we have only solid is present and rest of the remaining domain only gas is present.

So, this is only gases there, but if you use the Euler-Euler approach we lose the individual entity of the solids the individual entity of the discrete phase; why I am saying individual entity because each discrete phase solid is an individual entity ok. So, we lose that entity and we say that this is not the solid this is also a fluid.

Now, the fluid has a property that they can mix each other they can penetrate within each other. So, if you do that Euler-Euler simulation what will happen? You will not get this that there is a solid days a gas here or here this is only solid and this is only gas; you will get in this computational domain it will something like this and you will say that this have actually 30 percent solid say a number I am just throwing and 70 percent gas.

Why? Because they are inter penetrating continuum both are continuous, both are inter penetrating it means both will present everywhere; while in real domain what happens? That some places only a solid will be there, some places only gas will be there they will not penetrate with each other. Like if I am sitting here I have gas cannot or air cannot

penetrate inside me from this body it can go only through my nose ok, but it cannot penetrate through my skin or cannot penetrate through my body.

So, if I am sitting here it is only me no one else no one can else can come, but if suppose I am solving a Euler motion with me or kind of Eulerian equation for me or for any body what will happen? You will see that some places if I put a domain, I will you will say that say 60 percent of me is available, 40 percent of gas is available. So, in that way you will see that because we are now becoming continuous flow.

Now, if you are continuous I will be also present everywhere gas will also be present everywhere while if you think about this room where I am sitting right now; I am present at a particular location I am not present everywhere, but if I am interface if I solve interpenetrating continuum with a complete domain kind of a company; if I take this as a complete domain or complete room as one cell, you will find that week I will be presenting everywhere because I now becomes are continuous.

So, if I continuous I will be present in that cell I will be present everywhere. So, in that way the particles becomes of the fluid this discrete phase becomes interpenetrating continuum and you solve a continuum equation for both the phases and you assume that they can interpenetrate. So, what you are going to do? You solve as many question as many phases you are you are having.

So, it means if you have three phase; you are going to solve three the continuity equation, three momentum equation. If you are having two phase you are going to solve two continuity equations for both the phases individually and two momentum equations for both the phases individually and you will use the coupling to inter correlate this motion of both the phases.

So, we can solve two way coupling to see that how the motion of the particle say phase one is affecting the phase two; how the motion of phase two is affecting the phase one. So, you can solve one way coupling, you can solve two way coupling even you can solve the three way coupling or four way coupling, but for solving the four way coupling; you need to modify the equations, you have to include several terms and we will discuss that how to include that.



So, that is the Euler-Euler approach very widely used and why it is very widely used? Because you are solving very few number of equation; computationally it is not very very expensive. So, that is the reason it is widely used; so, like if there is a three phase present you will assume that in this room all the three phases are present now their fractions will be only different while it may possible say if I put a water into a glass here at this table then maybe this what will be possibility that water is only at this location at a particular location I am at a particular location of air is everywhere.

But if we will solve continuity or kind of Euler equation; you will find all three of us is presenting everywhere at the different fractions ok. So, that is two fluid model then come to discrete element model. Now discrete element model is very close to the language truck model what we do? We solve via the Newton's second law of motion for each individual discrete phase ok.

Once I say individual a discrete phase it means suppose there is just a solid bed; there is the individual phases will be each for each solid you will solve one Newton second law of motion. Then we solve one continuity equation, one momentum equation for the continuous phase say for gas phase ok. And then we solve the collisional part of this that how this particle motion is going to affect the motion of particles.

So, ideally DM model can accommodate all the four way coupling very easily and that is the major reason that why we solve the DM equations ok. So, you can have the collision equation we can have that how the motion of fluid is going to affect the motion of the particle; how the motion of particle is going to affect the motion of the fluid how the wave form because of one particle movement is going to affect the motion of the other particle.

How the collision of the particles is going to kind of affect the motion of each other. So, all you can solve here and that is called by the discrete element method; what we do here we solve one continuity and one momentum equation for the continuous phase and individual Navier Stoke kind of the Newton's second law of motion for the discrete phase. So, if you have say 10000 discrete phase available or 10000 particles available; what you are going to solve? You are going to solve 10000 Newton's second law of motion for those particles one navier stokes equation of momentum equation for the gas phase, one moment continuity equation for the gas phase of fluid phase.

So, you are going to solve 10002 equations then we also saw the collisional equation here. So, this and this difference Lagrange interact differences in Lagrangian track we actually do not solve the motion of the fluid; even if you want you can solve, but we do not take the particle collision into the account. Here we took their particle collision into their account; so, that is why it differs. So, suppose what we are going to now do if you think about the problem; if I have a 10000 particle in a fluidized bed I want to use the DM approach or D A model.

What I need to do? I have to solve 10000 Newton's second law of motion equation to track the motion of each other particles. Then to find how the collision of between the two particles is affecting their motion, I have to solve 50000; if I just assume that it is a two body collision and at a time only two bodies are colliding with each other 50000 collisional equations we have to solve; one continuity equation one momentum equation ok.

So, it means how many for 10000 particles you have to solve 10000 plus 5000 plus 2; it means 15002 equations. So, that is made this whole approach computationally very very expensive and that is the region that even now at industrial scale; with the current computational facilities we cannot do these simulations at industrial scale. Because think about the number of equations you have to solve simultaneously and that is why that ultimate wish which I have shown you need to be fulfilled understood understand how to couple these equations together or how to instinct the information from one set of model and use that information in the Euler-Euler simulation.

And then the last one is the fully resolved and fully coupled. So, each phases are resolved individually; each phases all the way of coupling we have taken here all the wages of interactions we are taking account. So, these all are the different modeling approach available, we will try to discuss these three modeling approach to we have already discussed earlier. We will try to discuss these two this three mainly and we will see that what equation we need to solve, what is the limitations and how to solve these equations? Ok; Now these are the modeling approach available if I see that if you see that if you move from the top to the bottom, you increase your complexity.

But your understanding of the physics is more is increased; it means if you move from the top to the bottom computationally you will be very very expensive or

computationally you will be more expensive as you move to the downward, but physics wise your understanding will be much better, you will be more closer to the real process condition or real process behavior and that is the way it should move. So, this is I will say more physics more expensive computationally once I say expensive; it is completely computationally expensive ok; more complex ok. So, once you move from the top to the bottom. So, that is the different modeling approach available and we will discuss about the different modeling approach in the next class.

Thank you.