CFD APPLICATIONS IN CHEMICAL PROCESSES
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Lecture 05: Introduction

Hello everyone, welcome back once again with another lecture of safety applications in chemical processes. I am Arnab Atta. We will continue with the basics, the introduction of the law of conservation of mass, momentum and energy that we started in the last class. So, in the last class what we have seen is that we will mainly focus on the three pillars of this understanding. One is the mass energy and

mass momentum and energy equations. And before that just quickly refresh your memory with the things that all the things the development or the derivations that are not shown here, you can find in the textbook the classical textbooks of any fluid mechanics, fluid dynamics or even the heat transfer textbooks. The point is that I told you earlier is that these governing equations are usually based on two reference frame can be based on two reference frame. One is the Eulerian, the other one is the Lagrangian framework, the Eulerian and the Lagrangian framework.

In Eulerian framework what happens you have a fixed reference frame which means you see a flow go through. your point is stationary. Say for example, you are standing on a platform of a railway station and you see the movement of coaches of a train. So, each coach you can consider as a control volume in the case of a fluid flow. So, the control volume is basically passing through a fixed reference frame.

So, that is your Eulerian framework. The other case that can happen the other reference frame is that if you are not on the platform and looking at the movement of each and every compartment or the coaches of the train. Other thing that you can do is that you can hop on each and every compartment and then locate its positions or you go through or you go along with the train. So, which means you are moving along with the same velocity or the speed of the train.

So, in the Lagrangian reference frame this thing can happen the framework is that the reference frame is moving with the same velocity of the liquid or the control surface. So, these two based on these two reference frame all these three equations all this conservation equations can be derived or are basically derived. As I told you for the single phase case from both the reference point that means, Eulerian Lagrangian the final expression of these conservation equations are identical. It differs there when there is a complex system or the multiphase system.

Also, the other important thing that you must remember is the continuum hypothesis for the basic equations in computational fluid dynamics. That means, here as I told you earlier we consider this the fluid that is flowing is a continuous fluid. And, in the last class if you go back to that if you cannot remember what is the continuum hypothesis of the continuous fluid, you can look into these expressions this explanation of these expressions that I provided last time. We also looked into the first equation that we took is the conservation of mass ok. We discussed its various components.

and then we went to the conservation of momentum equation. We started that at the last part of the last class. Now, coming back to this conservation of momentum. So, the conservation of momentum all the expressions that are here has usual nomenclature except the point that I already have mentioned here is that this term is the molecular flask of momentum rho g is the gravitational force and F is any external any other external body force per unit volume.

The first term that appears is the rate of increase of momentum per unit volume. The second term shows the change of momentum per unit volume caused by pure convection. So, rho u term is the convective term. So, it represents the change in momentum per unit volume imparted by convection. Then this two terms we have explained and now this molecular flux of momentum can be broadly categorized in two parts, one is the pressure force or the pressure term, the other one is the viscous stress term because both comes from the molecular flask of the momentum.

Now, the point is this stress tensor the viscous stress when we try to evaluate this or we have to estimate this to solve this conservation of momentum it has to be interpreted in terms of velocity. So, that the velocity field can be calculated in conjunction with the pressure field. So, now the equations that relate this stress term with the velocity term or the moment or the what we can say the motion of fluid. This stress terms by the equation that we relate this stress terms with the motion of fluid we call those as the constitutive equations.

Now, those constitutive equations or we can say those are the rheological equations constitutive equations or we say as the as the rheological equations of flow or maybe more specifically we can say the rheological equation of state. Now, this equation is valid for all the fluids, but there are different classification of fluids as you are aware of it that the fluid material varies depending on its nature and the broad classification that you see is the Newtonian or the non-Newtonian fluid. and we know that the fluids that follow the Newton's law of viscosity again although it is a Newton's law of viscosity that we are saying but it is essentially an empirical equation. So, which follows this Newton's law of viscosity which we call those are the Newtonian fluids and the others are the non-Newtonian fluids.

Now, inside that non-Newtonian fluids there are several fluids that again we will not discuss that those in details because it is assumed that you know or understand this term. So, the power law fluids there are Bingham fluids And, there are also time dependent shear stress fluids which are pseudo plastic, dilatant material etcetera those are there. Now, the point is this stress term this general deformation law of stress that we write usually is that tau ij that we write is

is Kronecker delta which means it is 1 if i is equals to j and is equals to 0 if i not equals to j. which is the vital parameter is the coefficient of viscosity and this kappa that we have is the coefficient of bulk viscosity. So, this is the transpose that you see and in most cases except for say the shock wave studies and in the cases of aqueous waves. with absorption and say the attenuation except these few cases usually this bulk viscosity is we mostly ignore that its contribution and then what it remains then only the first part of this expression. which is then used in the previous part here and again this is further plugged into this equation to get its complete form of the conservation of momentum.

Now, there are special cases along with this. So, this is the conservative equation where we represent the stress in terms of the velocity or the motion of the fluid. Now, in certain special cases this momentum conservation equations are simplified and when we have say the constant viscosity and say the constant density.

So, when this in this expression we have constant density and constant viscosity this equation this conservation equations is then famously called as the Navier Stokes equation. Now, that is the basis of this CFD applications because in most of the time we simplified our system considering this constant viscosity constant density system and then we apply Navier Stokes equations to solve or we model the system because again as we see here a complete full-fledged version of this cannot be solved analytically or even in the case of Navier-Stokes equations without further simplifications that cannot be solved analytically and that is the genesis of this CFD modeling approaches. where then we convert these partial differential equations to a set of algebraic equations by various methods that is called the discretization step. We will discuss that to solve this velocity and pressure field.

Now when again the system slowly gets complicated when we have other situations like the reactions multiphase system and etcetera the situation gets more and more complex. Now, the fluids that does not vary the does not go as per the Newton's law of viscosity as we said that those are the non-Newtonian fluids. And in those cases this contribution of say here this molecular viscosity usually is represented by a. apparent viscosity term or a property that relates this discourse the variation of the stress tensor with the motion of the fluid. Now, in those cases we call that as the effective viscosity effective viscosity term.

and that is a function of the your local stress and strain values that is a function of this local stress and strain values. Now, for the other or more complex non-Newtonian fluid it requires a different framework which is presently out of scope of this discussion here. So, we will not go into the details we will stick to this simplified thing where we will discuss mostly on the Newtonian part. Coming to the so, we have now discussed mass and momentum. Now, coming to the energy part the energy equation that we can have is for the law of conservation of energy that used to derive the transport equations for total energy.

what we can write for that in terms of enthalpy. If we consider H as the enthalpy, then for the conservation of energy. will have a form. So, for multiple species that is that species k that we discussed earlier also. So, what we have here is that H the enthalpy that we can define the total enthalpy is that m k h k which means

h k is your T reference to T C p k d t. So, where T reference is the reference temperature C p k this term is the specific heat of species k at a constant pressure q is flask of enthalpy the other are the conventional nomenclature that we have already seen. So, here what we have the first term similar to our previous understanding the first term is the accumulation of enthalpy. the second term is the change of enthalpy due to convection ok.

This is the third term change of enthalpy due to conduction ok. This fourth term represents the reversible change in enthalpy due to the pressure and this is the irreversible change due to the viscous dissipation. Here we have. minus sign missing ok. So, then what we have this term the sixth term the sixth term of this expression it means that the change of enthalpy due to the diffusive mass flux.

So, this is change of enthalpy due to diffusive mass flux. and similar to our previous understanding the last term is the volumetric source of enthalpy say chemical reaction is happening. So, there is a change in enthalpy of the system. Now, here the Q the flux of enthalpy that can be written in simple terms of temperature gradient by where k is the thermal conductivity of the fluid. So, this energy equation that you see which we have seen for each and every term it is in quite exhaustive terms are there, but here you see this equation cannot be solved in a standalone manner.

If you have to solve this expression for the enthalpy or its changes you need to know what is the pressure field as well as what is the velocity field. So, this term and this term these two are directly linked with the momentum expression that is here and this velocity term tau that you see. So, that is why when we try to solve a system to simplify by CFD model is that we try to do at first initially a cold flow simulation, which means cold flow simulation means without considering although system is having some reactions or some temperature changes etcetera. we try to model it in terms of simply just mass and momentum conservation without solving the energy equation.

So, that we at first have this velocity and the temperature field correct information. but it is not that accurate because this third equation I would say this conservation of energy as you can see is directly related or directly linked with that velocity and pressure field. So, that information comes here. this equation gets solved whatever the enthalpy is changed based on that if the fluid property changes those actually are again imparted or imparts their influence in the hydrodynamic flow or hydrodynamic simulation. So, this cold flow simulations by this term I meant to say that there is no reaction, no temperature change anything is happening which we can simply also say that the hydrodynamics of the system.

So, the simple hydrodynamics that means it involves the mass and momentum expression and then when we link that with the expression of energy and then other further equations are there to complicate the system that the transports of species the concentration changes etc. So, those in fact, like this conservation of energy are linked or has linked with the velocity and the pressure field you we need to know its expression of it fine. So, the point is now depending on the situations that we discussed in the last class as well that if we try to analyze the order of magnitude of each and every term we can understand its relative contribution. So, when which term is dominant if we can understand beforehand then we can simplify or we can neglect few of the terms in this expression and can simplify the system.

So, for example, for most reactive system most reacting systems the contribution of the energy that is released or absorbed by the chemical reactions usually dominates over the other term that originates from only pressure or viscous effects. So, in those cases the pressure or the viscous effect from these expressions can be removed or can be neglected can be dropped to simplify this expression ok. So, but in the case of say highly viscous flow even with the low heat of reaction, we may have to consider the viscous heating term. In those cases the viscous heating term may be dominant.

So, but these understanding these in these informations will come if we do the order of magnitude analysis if we can do and that will give us a less complicated form of the expressions less I mean more simplified form of the expressions which are easier to solve or easier to simulate. with lesser time. Because one thing you must appreciate that as we increase the number of terms in an expressions the situation gets more complex, the number of iterations of solving that equations is also increased. So, the it also increases your computational power demand. it becomes more and more computationally intensive.

as we increase those influences or if we do not simplify the system considering this which one is more dominant in my case or if we cannot anticipate that if we use this generic expression having all terms if we consider having equal significance in the system then in that case it would be more computationally exhaustive or intensive. So, simplification of governing equations are essential and in order to do that the thing that we should do is that when we can do is the non-dimensionalization of the governing equation or try to find out the non-dimensional form of the governing equation. If we do that then what it helps is that it gives us this form in terms of all non-dimensional number and few dimensionless numbers and this importance of the non-dimensional number of the dimensionless numbers are huge. It like Reynolds number you know which is very simple for you. is that when we say Reynolds number you immediately say it is the relative it gives us the relative contributions of the viscous and the inertia forces of the inertia to the viscous forces.

Which means if it is higher Reynolds number high means the inertia force is important the viscous force is less important. So, similarly once we non-dimensionalize this governing equation, it helps us to understand this relative contributions and accordingly the system can be simplified. But, again in most cases when we try to work with a new system which has not been explored in the research, we do not have any other option, but to completely consider the consider all the terms of the expressions. But, sometimes intuitively few terms are definitely neglected when we anticipate those are not important. So, these are the very basics of analysis.

this CFD course that I tried to convey. And in the next class what we will see this was simple non-dimensionalization and couple of non this dimensionless numbers and why those are important and how those help our governing equations in fluid, in mass, in energy.

So, with this I thank you today for this time and your attention. We will see you with the next lecture. Thank you.