CFD APPLICATIONS IN CHEMICAL PROCESSES
Prof. Arnab Atta
Department of Chemical Engineering
Indian Institute of Technology Kharagpur
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Lecture 04: Introduction

Hello everyone and welcome back once again with another lecture on the basics of CFD applications in chemical processes. Today we will discuss a few basic governing equations that are important or that are the cornerstone of the CFD modelling. So, those three that that are important that comes from the universal laws of mass momentum and energy. Now, mass momentum and energy

So these three universal law that we have to understand you are aware of it but still I will take you through this initial part because these are the basic thing that we will discuss again and again in the later part. Now, before doing the before going to the equations let me tell you that this fluid dynamics computational fluid dynamics in this thing there is a specific hypothesis that we consider inherently is called the continuum hypothesis. or very specifically we consider there is a continuous fluid exist which means now all the things all the materials and from a broader perspective consists of molecules and we also know the concept of mean free path between their collisions. Now the point is here in CFD the basic assumption what we do is this continuum hypothesis which means that the length scale of the mean free path.

of the fluid since we are specifically focused on the fluid dynamics I am just focusing on the fluid here. So, for the fluid the mean free path and the characteristic length scale. Characteristic length scale means characteristic length means typical domain dimension. So, mean free path mean free path of say the gas for the gas is in the order of 10 to the power minus 7 meter. For the liquid this is in the order of 10 to the power minus 9 meter or say minus 10

So mean free path for the gas is in the order of 10 to the power minus 7 meter and for the liquid it is 10 to the power minus 10 meter. The characteristic length signifies that through which these fluids are flowing or on which it is flowing. If it is a closed flow or a closed channel flow, characteristic length is the diameter of the channel or the hydraulic diameter of the channel. If it is open channel flow, it is the edge dimension, so that is why I mean first of Now this ratio you are aware that this mean free path length scale and the characteristic length scale is actually designated by a non-dimensional number called the Knudsen number.

Now, this continuous fluid inherently means that this mean free path is significantly small than the characteristic length scale in which it is flowing or over which it is flowing. So, which means the Knudsen number that is there. is much lesser than 0.01. If this criteria satisfies then we usually call this as continuum and say the specifically for the fluid case here we say the continuous fluid. and we safely apply the equations that we will now talk about in those cases.

And in fact, in the example in the last class that I told you about the reactors, there this characteristics length scale is used compared to this main free path. So, safely the CFD is applied, CFD modeling is applied in these cases. When we go to the microscale microfluidics or say the nanofluidics, then we have to be aware of this thing whether it is the liquid that is flowing you are considering for the CFD or whether there is a gas flow. a micro channel which means typical dimension 10 to the power minus 6 and look at this criteria for safe use of CFD ok. So, if there is a gas flow in micro channel

ok and you are possibly marginally safe if you are using a micro channel of say more than 100 micron. But if it is a say 1 micron channel 1 micron means 1 micron diameter channel and you are flowing gas phase through it that has a typical mean free path length of 10 to the power minus 7. This criteria is possibly is in fact would not be valid then and your CFD model would be looked differently or people will have doubt on your CFD model. So, and specifically now you consider the nano channels where the gas is flowing you cannot possibly use the CFD models there, but for the liquid case it is still the 10 to the power minus 10 because the nano thing is 10 to the power minus 9 meter.

So, again nano scale means if it is 1 nanometer or below that. CFD models are not useful or cannot be principally used. So considering these facts and the thing is that we will use it for the commercial applications where we have characteristic length scale of significantly larger and this criteria in most cases are usually valid. for the scenarios that we encounter in chemical processes. But as I told you if there is a nano specific or micro specific application we have to be careful before applying the CFD model looking into the validity of this assumptions.

Because all the equations that we will discuss and the fundamental the cornerstone of the CFD that is the Navier Stokes equations is based on this continuum hypothesis. there are also different two different say reference based on which the governing equations can be derived. We will not go into the derivations as such of these equations, but the point is we will look into the form of those equations and the point is the reference frame based on which it is developed. The point is there also you are aware of two reference or the approaches based on which the governing equations are developed. One is called the Eulerian framework, the other one we call the Lagrangian.

Eulerian framework and Lagrangian framework to derive this basic governing equations. Now the point is that these two approaches although it takes a two different rules, but when we solve it for the single phase system or when we derive for the single phase system it results in the same form of equations. are the same equations same governing equations. But these reference frames creates or say I would say more critical situation when it comes the multi phase flow system. We will see into that we will look into that because modeling multi phase flow and say turbulence

based on these two system we will when we look into this individual part the turbulence and the multiphase flow will see that but the point is these frameworks yields differently when we have those two scenarios specific scenarios than the single phase case so if we look into the conservation of mass if we look into So if we look into the conservation of mass we write the conservation of mass in the form of mass fractions of the species that are involved in a system then the molar concentration because there is a flow. So, the flow property may vary throughout the compositions and with temperature. So, the mass conservation equation say for any species K we can write it in the form

So, where we look into this as t as time, rho as the conventional meaning of it, rho is the density, m k is the mass fraction of species k. So, m k is the mass fraction of the species K, capital U is the fluid velocity. So, the first term the first term that in this expression that is here this represents the accumulation of species k in the system the second term that we have here. So, this is the accumulation part

The second part the changes of species k in the system due to convective motion or due to convection. So, this is the convective part. So, changes of species k of its mass fraction due to the convection part rho u. Now on the right hand side of this equality the first term here is the change in species mass fraction due to diffusivity or the diffusive flux and this diffusive flux is j k. this S k is the source term of species k, the net rate of production of species k in the system per unit volume.

So, this is the source term species k per unit volume. So, the volumetric source can be a rate of production or consumption due to the chemical reaction or net say exchange of species in the system with the other phases the source term this is how it is interpreted. So, again this net the source of the species K that can come from the this rate of production of species K or its consumption from the system due to chemical reaction or say the net exchange of species K between different phases in the system that the species K goes from liquid phase to gaseous phase or it comes from the gaseous phase to liquid phase in the reaction.

Now, for the non reactive system if just simple mixing is happening and the flow is there So for the non-reactive and also for a single phase flow, where there is no chance of having this the net exchange of species K between two phases, even if the reaction is not happening. So single phase non-reactive system, the source term is not there, doesn't exist. for the reactive system multiphase system the source term may exist depending on the situation. Now the point is.

In this case this system it can be solved for the species the mass fraction of species to know where the concentration is if we know this velocity field. So, this is written in vector form. So, this U the capital U is the velocity field if it is known then the equations can be solved easily. but that does not happen in a system you also do not know how the velocity is changing or what is the dynamics that is happening. So, that is why it is solved with the velocity field equation which is essentially the momentum equation.

Now, before going into that we have to understand that there can be several scenarios where sometimes the convective part is dominant where the diffusive part is dominant. And that just based on the order of its magnitude analysis one can understand that whether in my system I have strong diffusive flows the convective part is less important or not that significant compared to the diffusive flux. Then what usually is done again now here comes the model simplification that these terms or this term depending on its dominance, the dominance of the convective part or the dominance of the diffusive part is taken out from the equation.

If diffusive flux is dominant what we consider then? Diffusive flux is dominant then we consider this convective part is absent and this is the approximation that we do to simplify the system or if the convective part is important. if the convective part is important then we may not consider diffusive part and then we go for a simplified system or the simplification of this governing equation. Now, the point is that the diffusive flux is composed of diffusion due to concentration gradient which more specifically or as a chemical engineer we can say the chemical potential gradient

It also composed of diffusion due to thermal effect and diffusion due to pressure and any other external sources. So, now again so, depending on these parameters that you will now understand that it has several parameters. The diffusive flux that I told you that it can be due to the chemical potential gradient thermal gradient pressure gradient any other external forces depending on whether your system has any of these or all of those then you have to consider your system accordingly and you have to model this diffusive flask accordingly or if those are absent in most cases this absence of these are this external forces are there external force is not there.

So, in most cases this J k is or say if I consider the combined effect of this where this term dKm is the diffusion coefficient for species K in the mixture and this term is the thermal mass diffusion. of species K. Now, again what is typically seen that this thermal mass diffusion is mostly negligible in most cases or very small compared to this diffusion mass coefficient diffusion or mass diffusion coefficient. And further so, this term is then simplified by neglecting this part and this is then plugged in here and we get an overall system that looks like.

for any species k in the system this is a simplified version of the mass conservation and when we take the summation of species all the species then it essentially for the overall system what we write usually So when we have mass conservation for all the species this is the mass conservation equation that is solved in the CFD modeling part where K is the number of species that we have. So the first term again presents accumulation The second term is the contribution that comes from the convection and the third term represents the summation of sources for all the components. It is the source term for all component.

For single phase case again for single phase a simplified system the source of all components the summation of all components will be 0 since there is there cannot be any net generation or destruction of mass and then this term disappears for that case and becomes 0. So, this is the mass conservation equation that we see. Now, as I told you this can be solved individually if we have the flow field known to us or the velocity field known to us, but it does not happen and that is why we solve it along with the conservation of momentum equation. Now, this conservation of momentum equation how it comes please refer to the standard fluid dynamics textbook be it Birds and Stewart, Lightfoot, Fox, McDonald and everything.

You will see that the governing equation is composed of velocity and pressure field and has a form in vectorial where this pi that I have written here is the molecular flux of momentum. g is the conventional rotation that you have the gravitational acceleration and f is the external body force per unit volume. all other notations as the conventional meaning and you have seen it earlier.

So the physical interpretation of this momentum equation is that the first term is again the rate of increase of momentum per unit volume that you see here the rate of increase of momentum per unit volume. Second term is again the convective term that we see that the change in momentum per unit volume. caused by convection this is the convective part. And then these two are the gravitational force per unit volume and as I already told F is the any other external force per unit volume. Now, this whole third term of this expression

represents this as I said the molecular flask of the momentum or the molecular contribution which means this includes the pressure and the viscous force per unit volume and usually this is given as where P is the pressure. and tau is the viscous stress tensor. Now, the point is these equations you have already seen ok. We will not go into the details of how it is derived, but we are looking into a form that is familiar to you and we are explaining it that which term represents what and what when some can be neglected.

Now as I told you here in this case this third term represents the molecular contribution that comes from the pressure and the viscous part. So, if your system is having the inviscid flow which means the viscosity is negligible then the contribution of those term does not appear in the modeling equation. ok and you know what is that equation. Similarly, if the velocity is extremely high ok and in that case you have a different scenario and we will see in the next class that which term we can then neglect. Because here also you have a comparative understanding if your diffusive flask is dominant or a convective part is dominant, then you can simplify the system that is all.

It is not necessary that that has to be done. A system if the order of magnitude is significantly different in this diffusive or the convective term, then one can be neglected. It is not necessary that it has to be neglected. Both can coexist in several flows. And in those cases this full equation we have to solve or all the terms of this equation we have to evaluate.

So, I will stop here today we will take up this discussion on the conservation of momentum equation in detail in the next lecture where we will see the energy equations further and also we will conclude this introduction basic introduction parts by touching upon the boundary conditions as well. With this I thank you for your attention and hope to see you in the next class. Thank you.