CFD APPLICATIONS IN CHEMICAL PROCESSES
Prof. Arnab Atta
Department of Chemical Engineering
Indian Institute of Technology Kharagpur
Week-02

Lecture 07: Fundamentals of Fluid Flow & Heat Transfer

Hello everyone, welcome back with another class on CFD applications in chemical processes. We are continuing our discussion on the fundamentals of this governing equations for fluid flow heat transfer and mass transfer. So what we have seen in the last couple of classes is that how those governing equations look like. We will continue on that. Also, we have seen the importance of non-dimensionalizing the governing equations and a few non-dimensional numbers and their importance and why we need those the information on the non-dimensional numbers.

So, along with those equations now there is definitely we require the non-dimensional numbers to understand the relative contribution of the forces, if there are forces or the contributions from different terms. So, that we can simplify our governing equations wherever or whenever possible. But, along with those equations we also would need fluid properties or the material properties to be evaluated sometimes, if those are not specifically known either by experiment or from their property table. Now, the point is those properties the fluid properties generally are the function of temperature pressure and the composition if there is the multi component fluid.

So, say for example, density So, for example, the point of density, density if there is say multi component fluid that is flowing, we know the pure component substance density ok. But depending on the concentration or the mass fraction of the component that are present in that multi component fluid, we may have to evaluate its mixed property. So, generally we use this mixed property and, but those mixed properties are either you have to experimentally evaluate all the time whenever you do that or you can estimate by this kind of expressions or the equations. So, again this ρ_k is essentially the function of pressure and temperature.

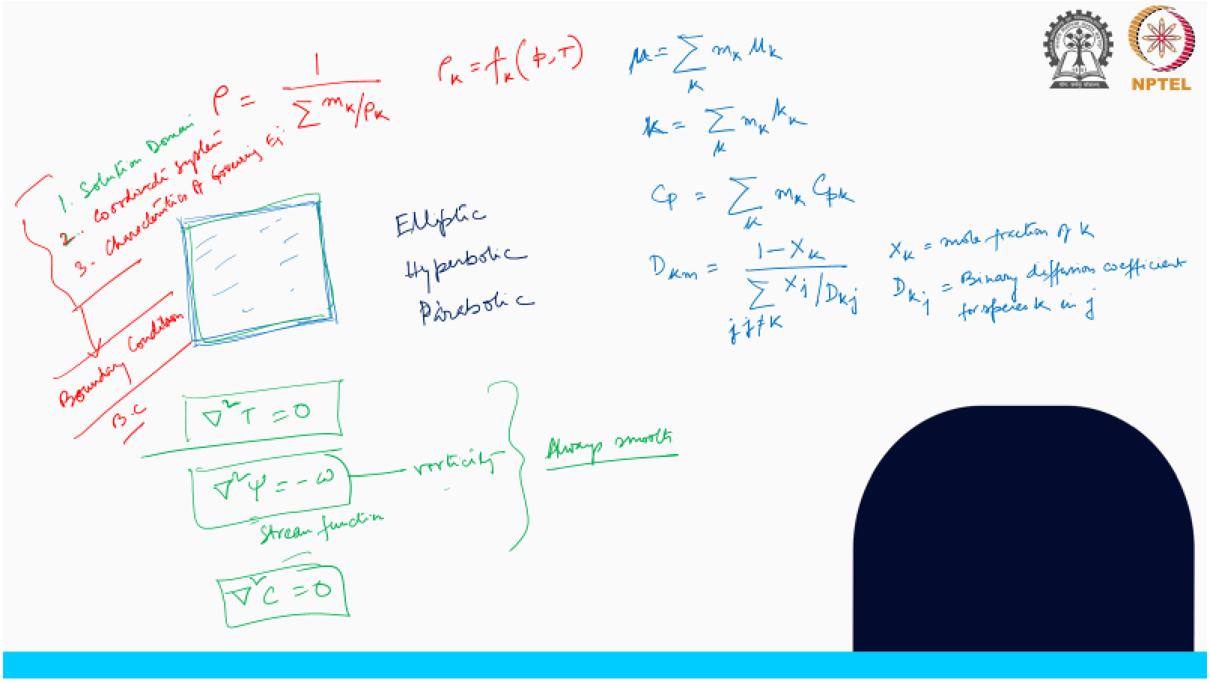
So, this m_k we have seen earlier this expression is the mass fraction the mass fraction of the species k. The pure component substance the pure component for k density is ρ_k. So, for such any species if there are multiple species we can combine those this ratio and get the density of that multi component fluid. Now for ideal gases this estimation of ρ is also easier because that we can relate with the molecular weight of the species K temperature operating temperature operating pressure and the universal gas constant that PV = nRT from that we can find out the relation of the ρ and subsequently use in the expression. And, for the non-ideal cases again you are aware of equation of state, various equation of states are available Van der Waals, Peng–Robinson, and Soave all the equations are there. So, from that you also again can find out this the pure component species, their densities depending on the temperature, pressure and the non-ideality.

one can find out this mixture properties. Now, this there are several alternate formulations of this kind of mixture properties say for example, instead of mass fraction one can also use the molecular say the mole fraction But, most of the time it has been seen that this mass fraction concept works pretty well with the mixture properties and to understand the mixture property. So, the for example, the multi component flow It has been customary that we use this mixture properties and mostly with the mass fraction weighted average of the individual component for say other properties like viscosity, thermal conductivity or say specific heat etc.

These components are also possible to be evaluated from the kinetic theory of gases, but will not go into those kind of formulations or say how do we get it. It is possible to get that and usually the mixture properties of say the other important fluid properties for example, mu the viscosity the mixture viscosity that we typically evaluate based on such kind of a expression. That means, the mass fraction weighted average of the pure components that are present there. So, similarly for K, now these are important because

So, this properties not only the governing equations you said, but when you have to solve those governing equations you have to fit in the fluid property that what kind of fluid that is flowing and simple water or maybe polymeric fluid etcetera. When you define that it actually this your CFD code or the CFD model understand by the fluid properties. The changes in fluid properties is identified because it does not really understand that water is flowing. It understands that the viscosity of water and the density of water, these numbers, these liquid properties that they are present, that you are giving in. Accordingly, it understands that this fluid is flowing.

So, similarly so, this is the K that I and this is μ and for Cp similarly what we can have is the Now, for the mass there is an important parameter that is the diffusion coefficient and it is not such straightforward method that is used to find the diffusion coefficient or the multi component mixture. So, in such cases the for the mixture of say ideal gases. because non-ideality introduces several complexity and several empirical relations are available those comes by the research. But for the ideal gases mixture the diffusion coefficient in a mixture are usually estimated by

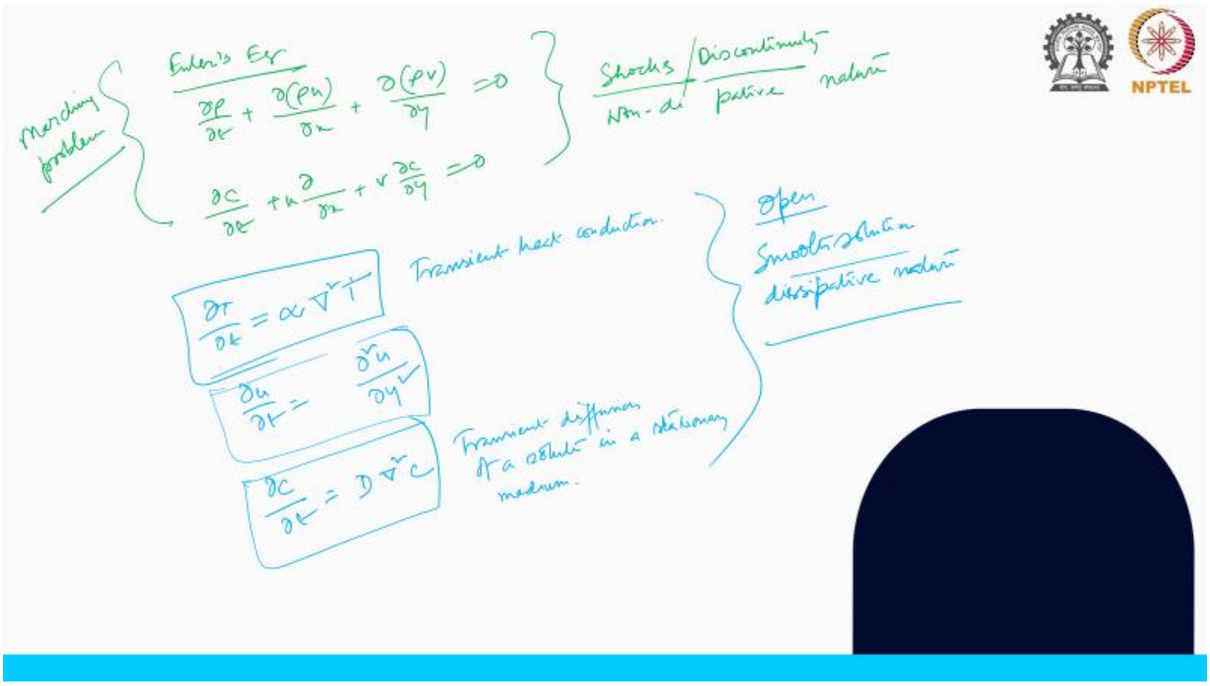


for all j's except when j is not the kth component for all the component. So, where this x_k is the mole fraction of component k and D_{kj} is essentially binary diffusion coefficient for species K in J. So, this is for the this is how? one way you can estimate instead of doing experiment to find out this parameter. If you know this pure component binary diffusion coefficient of species K in J and you have a multi component ideal gas mixture.

So the typical values that you find for the other properties usually comes from the experiment or if it is not ever I mean is there from the experiment either you have to estimate that or you can find out in several reference book handbook that are available to find those material properties. Now, the important thing is that. along with this material property. So, first of all you have developed the governing equations, you set the material properties, but the point is that to solve any partial differential equations because we mostly are dealing with the partial differential equations you have seen the patterns. These partial differential equations when we try to solve we need the boundary conditions or the initial conditions or maybe both sometime. So, the point is this boundary conditions becomes or the initial conditions that you have to set for the problem or for the model are extremely important.

Now, the point is the solution domain for example, you have a problem statement and for which area this model will be applied that has to be demarcated by this kind of line in 2D or 3D called the solution domain that my governing equations would be solved inside this area that is the solution domain. So, this solution domain actually demarcates from the surrounding ok, the area of interest is your solution domain. Now, this solution domain requires this boundary conditions that how it is interacting with the environment or the surroundings. So, that formulation is extremely important and understanding of those boundary conditions the suitable boundary conditions that would actually reflect the right physics identifying that is extremely important.

So, this solution domain coordinate system in which you have developed the equations And the equation characteristic because which also I will discuss in couple of minutes that this partial differential equations are broadly categorized in three different type. The nature of the partial differential equations can either be elliptical, hyperbolic or the parabolic. Generally speaking or in a classical way. And those characteristics that means whether it is elliptical, whether it is hyperbolic or parabolic, those characteristics I mean gives us an insight that how the solution or the solution procedure would behave.



So, solution domain, the governing equations, the coordinates of the governing equations in which you have developed and these characteristics of the governing equations. dictates that how this boundary conditions or influences how this boundary conditions nature would be or you should be taken into account. So, usually as I mentioned that we can have the nature of the any classical say the partial differential equation category are say the elliptic in nature ok. So, the elliptic hyperbolic or parabolic.

These are the category we have seen we have studied earlier also and I am not going into the how you determine because that you determine looking at the expressions finding at the eigen values of the matrix and all. So, we will not go into that I presume that you know that what are these elliptical hyperbolic and parabolic. form of the partial differential equations or how to identify. But at the same point I must mention that in the CFD course or this in the CFD modeling or any complex system there are governing equations which are of mixed type and easily cannot be identified. But we are currently talking about say the classical cases.

Say for example, the elliptical governing equations in heat transfer you would find say the form the governing equations that possibly you have seen this kind of a form of the governing equation. which is the steady state heat conduction in solid without any internal heat generation. So, the you can think of this is the parabolic sorry the Fourier's law. So, the elliptical form of the governing equation in fluid also you can have where this psi is the stream function omega is the vorticity.

So, this kind of governing equation would appear if you have creeping flow around an obstacle and where inertial terms are negligible. So, steady incompressible 2D flow that represents stream function and velocity formulation where you have this the stream function and the vorticity. In mass transfer similar kind of the form that you may find is this. which is the steady state molecular diffusion in a stagnant media without any reaction which is the Fick's law. Now, the point is in this elliptical equations information propagates in all three dimensions simultaneously.

The solution domain is therefore, we consider as a closed domain and the solution the resulting solutions are always smooth ok. However, if you look into the hyperbolic partial differential equations looking into the aspects into the different aspects say the heat transfer or say fluid or mass transfer in fluid we have a very popular expression that is your Euler's equation. say in 2D the inviscid Euler equations for continuity.

If we look into that so compressible look we see that the compressible inviscid flow that can appear in shock waves or acoustic waves. In mass transfer this kind of expression you would find which is So, convection dominated mass transport without diffusion. The point is such kind of expression the equations which are hyperbolic in nature. The information propagates along a characteristic direction with finite speed.

Which means these equations are usually solved by marching technique with time ok. So, and such solution may contain shocks that means, discontinuity ok because they have their non-dissipative nature of this expression. ok. And the other form that you can find is the parabolic form, the parabolic form of the this partial differential equations and you have a popular expression here for say heat transfer.

that you have the Fourier's law transient heat conduction. The examples that in future we will see the heating or cooling of a metal rod that is exposed to environment and if the environment is having lower temperature it would cool, if it is the higher temperature it would be getting heated. for fluid mechanics the example of this classical nature of parabolic expressions would be say the transient boundary layer formation okay so this usually appears say when you suddenly move a plate in which a fluid is stagnant so in such cases the transient boundary layer formation cases you find this kind of a governing equation and for mass transfer you may find that the transient diffusion of a solute in a stationary medium. So, in case in these

The solution domain in contrast to the elliptical where we consider as closed it is we consider that the solution domain is open, but it always results in smooth solution due to their dissipative nature. So, what we have for the elliptical nature of this characteristics of the governing equation, we considered those as the closed domain and we always have the smooth solution. In parabolic cases we also have the smooth solution, but we consider this as the open not the closed one, but we also have here similar to the electrical cases the smooth solution, but in cases of the hyperbolic nature those are here those are the marching problems or marching can be solved by the marching process.

And accordingly this information helps us in choosing the proper boundary condition or sometimes it influences the choice of the boundary condition, so that the solution gets converged. Now, the kind of boundary conditions we will discuss now, again depending on the solution domain I told you again it is 1 is the solution domain, 2 is the coordinate system, in which you have developed the governing equation and the characteristics that we just discussed of the governing equations. this all these three boundary conditions. So, in the next class we will discuss this details on the boundary condition that what are the typical boundary conditions there as I told you that it is not necessarily that any developed governing equations the partial differential equations you can categorize it either in this three way that is elliptical parabolic or the hyperbolic.

It is impossible sometime because of the complexity of the problem. But usually there is a standard state of boundary conditions that are mostly used and for as the situation gets complex for example, the multiphase system, multi component system with different volatility etcetera, we will have complex boundaries condition. But, what in the next class I will discuss a typical set of boundary conditions that are popular and helps us in setting up the problem that we will then start solving it after knowing the computational technique. So, with this I will stop here today and I will come back in the next class with the details of the boundary condition. Thank you.