

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 06: Fundamentals of Fluid Flow & Heat Transfer

Hello everyone, welcome back with another lecture in CFD applications in chemical processes. In the last lecture, I discussed about the importance of non-dimensionalization of the governing equations or the basic equations that we have seen for mass, momentum and energy. So, for a typical say, now how do we do at first the non-dimensionalization? For that we have to at first find out a characteristic length scale and the time scale because all these that we have seen are essentially based on this velocity pressure field which has and velocity and pressure and viscosity and other things which has the elementary unit or elementary dimension that relates with the time and the length scale. Now, this characteristic dimensionless number that if we try to find it, it is possible for us to appreciate the relative importance of the terms or relative importance of the various interaction that happens in a process.

Say for example, convection, diffusion, reaction etcetera its relative contribution in the process. A typical non-dimensional form of a governing equation for any variable say ϕ if we consider say for any variable ϕ if we consider that becomes. Now, this r represents the characteristic values or the reference values We will come to that, let me finish the form. So, r this superscript r represents a reference value.

$\left(\frac{\rho_r \phi_r}{k_r}\right) \frac{\partial}{\partial t}(\rho\phi) + \left(\frac{\rho_r U_r \phi_r}{L_r}\right) \nabla \cdot (\rho U\phi) = \left(\frac{\Gamma_r \rho_r \phi_r}{L_r}\right) \nabla \cdot (j\phi) + \left(\frac{\rho_r \phi_r}{k_r}\right) S_k$

$\Gamma_r = \text{effective diffusion coeff. } \phi$
 $k_r \rightarrow L_r/U_r$

$\frac{\partial}{\partial t}(\rho\phi) + \nabla \cdot (\rho U\phi) = \frac{\Gamma_r}{U_r L_r} \nabla \cdot (j\phi) + S_k$

$Re = \frac{L_r U_r}{(\mu_r/\rho_r)} \rightarrow \Gamma_r$

$Pe_{heat} = \frac{L_r U_r}{(k_r/\rho C_p)}$

$Pe_{mass} = \frac{L_r U_r}{D_r}$

Mass \rightarrow Molecular diffusion coeff.
 Momentum \rightarrow Kinematic viscosity of fluid
 Enthalpy \rightarrow Thermal diffusivity of fluid

$Re \uparrow$
 $Pe <$
 $Pr -$
 $Sc -$

Euler's Eq.
 Creeping Flow

High Speed Flow
 Diffusive Flow

Small Re

Peclet No. Prandtl No. (Pr) - Thermal
 Schmidt No. (Sc) - Momentum
 mass Diffusion

or the reference characteristics value that we use to make this thing or the equations non-dimensional. Whatever the term that does not have this superscripts are already non-dimensional that we have to consider for this expression. So, gamma this is the capital in upper case gamma, gamma r is essentially this effective diffusion coefficient for variable phi. So, if we have a characteristics time scale say this tr and we define that with the ratio of characteristics length to the velocity that means, L_r/U_r or essentially it is the other

way Then and if we put this into the expression in this non-dimensional form the generic form for any variable general variable ϕ what we have then.

that this is the non-dimensional form or the dimensionless form of that expression the governing equation that we have written earlier. Now, this non-dimensional form contains this dimensionless parameter and all other symbols that you are seeing are non-dimensional in this case. So, this term that we have here now, this is a non-dimensional term that appears here for any general variable ϕ and this effective diffusion coefficient that we have Γ_r this will be different based on the parameter that we choose as ϕ . Say for example, if we have say the mass fraction equation, if we have the momentum expression and if we have the enthalpy.

this effective diffusion coefficient in this case will be molecular diffusion coefficient. In momentum case it is the kinematic viscosity term. and for enthalpy this is the thermal

diffusivity of fluid. So, this Γ_r will take these forms depending on what ϕ or what which one as ϕ we are taking into consideration. If ϕ is mass fraction Γ_r becomes molecular diffusion coefficient, if this is ρu that is the momentum term.

then it becomes the kinematic viscosity of the fluid. If this is enthalpy that we have seen earlier, then this γ_r becomes the thermal diffusivity of the fluid. And as those changes this non-dimensional parameter or the dimensionless parameter becomes 3 different non-dimensional number. So, if we consider this in this case as the now coming back to this thing. So, if we now consider one by one say for the mass cases if we consider this is the mass fractions that is the happening and if we consider momentum and enthalpy.

So, this Γ_r becomes the molecular diffusion coefficient kinematic viscosity of the fluid and the thermal diffusion thermal diffusivity of the fluid. Now, we know the Reynolds number ok. Now, Reynolds number is interpreted as the ratio of convective transport to the diffusive transport or the molecular transport of the momentum. That means that we say that for the Reynolds this is the kinematic viscosity of the fluid μ by ρ . So, what we see here that this term in the case of momentum or the conservation of momentum it becomes 1 by Reynolds number.

So, this is the point that helps us in simplifying this momentum expression. How? Because as we can see that this Reynolds number Here, based on the characteristic length scale and the velocity scale that we have seen here with the reference number that is characteristic length scale L_r representative velocity U_r and this is your contribution that comes from the viscous term. So, convective term by the viscous term from the standpoint of the reference values which indeed is 1 by Reynolds number that we see here because this is the term that is Γ_r when it comes for the momentum case as we have seen that this Γ_r becomes kinematic viscosity of the fluid. So, what happens?

for the momentum if we consider now this equation it shows that if we have a very high Reynolds if the Reynolds number or very high speed flow is extremely high. So, very high speed flow that means, superficial velocity is very high Reynolds number is very high this term 1 by Reynolds number of the reciprocal of the Reynolds number becomes or tends to 0. That means, this diffusive term contribution the contribution from the diffusive term can be neglected if this scenarios of such high speed of flow occurs in any situation. So, if your system if in your system if you anticipate the Reynolds number is very high in that case to simplify the momentum expression you can drop this diffusive term.

go for the simplification of this momentum equation and solve it or model accordingly. Now, in such case the momentum equation this Navier-Stokes equation eventually is called the Euler's equation in case of very high speed flow. when you neglect the diffusive term diffusive plus when you neglect it when you do not consider those. Now, the other extreme is that you have an extremely say small velocity. or say very low velocity of fluid that is flowing through the system that can happen at very small scales micro scale, nano scale and etcetera.

And in those cases if you have very low velocity of the fluid your Reynolds number is very low in that case very small. So, small Reynolds number what you will it will do in this expression that if we see then in that case this diffusive term becomes dominant and your convective contribution or the convective part its contributions can be neglected. and then this Navier Stokes equation eventually drops to the creeping flow expressions. We call such low velocity flow as the creeping flow for the small Reynolds number cases very low Reynolds number cases we call that as the creeping flow expression fine.

Now, in case of say enthalpy and mass. So, we talked about the momentum case in case of enthalpy and mass when this becomes thermal diffusivity and molecular diffusion this non-dimensional number essentially becomes. So, in case of heat we have So, it is the thermal diffusivity that we see and essentially it becomes the Peclet number like the Reynolds number that we have here it happens to be the Peclet number again the spelling is Peclet number. We know this thing we have seen it earlier in the fluid mechanics fluid dynamics or the transport phenomena.

Similarly, for the mass it is the Peclet number for mass and it becomes by the diffusive term the molecular diffusive the molecular diffusion coefficient. In both cases we call this as the Peclet number, but when we divide this by the Reynolds number So, when the Peclet number we divide this with the Reynolds number, then what we get is the Prandtl number for the enthalpy case and Smith number. So, if I write it So, Prandtl number is the ratio of momentum diffusivity to the thermal diffusivity.

Smith number is the ratio of momentum diffusivity to the mass diffusivity. So, how many non-dimensional number we have seen now starting from the Reynolds number, Peclet number, Prandtl number and Smith number. this Peclet number are both used for heat and mass Prandtl number. So, when we divide the Peclet number by the Reynolds number we get for thermal case or in case of thermal properties we get the Prandtl number and for the mass we get the Smith number. Now, these are extremely important these numbers actually

are very important just because or the by the logic that I explained earlier in case of the momentum case.

Similarly, based on these numbers when you get to know these numbers, these numbers would tell you the relative contribution of these terms. So, in case of high Prandtl number cases your momentum diffusivity is higher you can possibly think of dropping the thermal diffusive part of the expression and make your model simplified. It is all about making the model simplified. So, that we can solve those quickly rapidly and in a less computational intensive way.

So, this non-dimensional numbers gives us or in a nutshell this non-dimensional numbers if we try to analyze this, this gives the relative contribution of various transport and generation mechanism and we need to know this beforehand that will make our life simpler. So, and also there are certain cases as we move along we will consider those or we will talk about those on a case by case basis, but those comes with an experience and lot of trial and error the typical general recommendation. One thing you will see in the throughout this CFD modeling part of the course that there or in fact in general cases that any problem by CFD model can be solved in various ways if you are given a problem in CFD itself there are various methods by which you can solve that problem the point is what you want to achieve or what is the wish list from that problem. What you are trying to achieve? What is your desired goal?

Setting that this CFD methods changes or you have to adopt different strategy in this modeling process differently. There is no one unique method that we can assertively say that this is the only process by which this process or a given thing can be modeled in CFD. So, what is the best process in CFD if someone ask or what is the best method to solve this problem for that the counter question would be that what we are trying to achieve or what we are trying to see what is my goal. Based on that with list we have to adapt the base strategy to solve that problem effectively and efficiently without losing accuracy by several simplifications. Simplification is good to have rapid simulation or the rapid result, but too much of simplification can deviate or does not provide the actual physics the insights in the from the problem.

Now, similar another point is most of the problem that we will discuss or are typically taken in the CFD problem can be solved in the Cartesian and the cylindrical coordinates. Now, this governing equations has to be modified or has to be taken into proper in the with proper modifications, we have to write it if we change that coordinate system that is another

thing that we have to keep in mind that along with the Cartesian coordinate and cylindrical system ok. There are also that in radial coordinates also you can represent this governing equations and if needed you have to solve that. So, but as I told you in most cases we solve this problems in the Cartesian and cylindrical coordinate because that surfaces.

If not we have to go for the other coordinates other coordinate system. Now, continuing on this non-dimensional number along with this 4 non-dimensional number that we have seen is the Reynolds number, Peclet number, Prandtl number, Schmidt number. There are few other non-dimensional number that I want you to recapitulate is that Nusselt number. Now, these numbers are extremely very important Nusselt number or Sherwood number in case of one is for the heat transfer cases one is for the mass transfer cases.

So, Nusselt number or the Sherwood number that gives you the ratio of total transfer to the molecular transfer this ratio be it for the energy or for the mass. So, this is for the energy this is for the mass this is the analogous non-dimensional number just like the Prandtl number and the Schmidt number. for reaction system for reactive system you will hear or you have already seen a number called the Damkuhler number ok. The Damkuhler number gives you the ratio of convective time scale to the reaction scale and the ratio of I mean it usually represents the ratio of convective time scale by the reaction time scale the ratio of these two or say or in other words it can also be represented as the convective transport and the rate of generation due to the chemical reaction.

There are numbers like Euler's number. Euler's number is represented by ρ by sorry p by the ratio of pressure force to the inertial force. If your system has significant gravitational force, then there comes another number is called the Froude number. the ratio of inertial force by gravitational force. If surface phenomena, the surface tension force or the surface forces are important in your problem, then another dimensionless number in fact, the dimensional number that helps you to understand the relative importance is the Weber number, which we write like this.

where γ is the surface tension which gives us the ratio of or I can say inertial force to the surface forces. For heat transfer cases there is Lewis number ($Le = k / \rho C_p D$). The ratio of to the mass diffusivity. So, the point of showing all this dimensionless number is to make you understand that if you find out this non-dimensional number from your governing equation and if these numbers are linked with your governing equations, then relative importance of these forces

Cartesian -
Cylindrical -
Radial ..

Re
Pe
Pr
Sc

Nu - Energy
Sh - Mass

Da - $\frac{\text{Convective time scale}}{\text{Reaction time}}$

Eu - $\frac{\rho}{\rho_w}$ - $\frac{\text{Pressure force}}{\text{Inertial force}}$

Froude No. - Fr $\rightarrow \frac{U}{\sqrt{Lg}}$ $\rightarrow \frac{\text{Inertial force}}{\text{Gravitational force}}$

Weber No. - We $\rightarrow \frac{U^2 \rho L}{\sigma}$ $\rightarrow \frac{\text{Inertial force}}{\text{Surface force}}$

Lewis No $\rightarrow Le \rightarrow \frac{U L}{\alpha}$ - $\frac{\text{Thermal diffusivity}}{\text{Mass}}$



can really be understood if you have those values. And accordingly the terms can be dropped neglected or may be considered rigorously based on these values. So, the importance of non-dimensionalizing governing equations and the non-dimensional numbers that we have discussed in details today. All the details, all these things in much greater detail if you are interested can look into the reference book that I have already shown you or in the traditional textbooks that I always iterate or reiterate is that you can go to the Bird Stewart Lightfoot, you can look into the Fox McDonald for the fluid mechanics textbooks. So, you can go into the incorporated unit Hollman in when comes for the heat transfer and for the mass transfer also there are several textbooks that you can easily go and look into these numbers their importance in a more greater way.

So, in the next class, we will continue on this, this fundamentals of fluid flow and heat transfer. We will see couple of simple thing. Again, these are kind of a refresher part before we go into the techniques of solving such equations. With this, I thank you for your attention and have a joyful day.