Computational Fluid Dynamics

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Lecture – 20
Equations governing fluid flow with chemical reactions

In last few lectures, we have derived the governing equations of fluid flow and we have derived this specifically for the general case where there may be chemical reactions that may be happening and there may be heat transfer and mass transfer that may be happening in this and in the within the fluid continue. So, in today's lecture which will take as a tutorial, we will just take a deep breath and then try to write down all the equations and then see what kind of equations that are there for us to solve numerically. So, we will write down all the governing equations that we had derived in the last few classes, and these equations comprise the mass balance equation, the momentum balance equation, the energy balance equation and in the case with chemical reactions we also have to have the species balance equations.

In all the lectures that we have been dealing with, we have started out with the Cartesian coordinate system and somewhere it is some point we have also put down the equations in vector form. In today's class, we will start with the vector form and then so that it is easy and compact for us to write them down, and if you want you can go back to the previous lectures and then write the equivalent Cartesian coordinate system form for easier understanding. So, we will start with the equations governing fluid flow.

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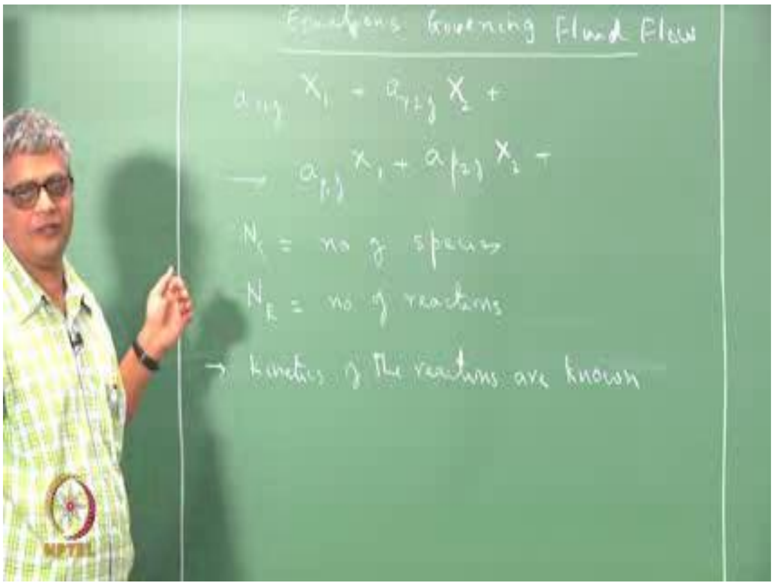

We are considering the case of reacting fluid in which you have a homogeneous reaction which is given in a stoichiometric way as like this, we have a r 1 j x 1 plus a r 2 j x 2 plus so on these are the coefficients stoichiometric coefficients of reactant 1, reactant 2, reactant 3 and so on in the jth reaction. So, we are looking at a large number of this reactions which may be happening in which species x 1, x 2, x 3 and so on are participating as reactants and these are getting converted to products ap 1 j x 1 plus ap 2 jx 2 and so on here.

So, in a given system of chemical reactions having ns number of species, participating in nr number of reactions, in this sometimes some of the reactants may appear as reactants and sometimes they may appear as products. So, this is a general scheme here and in this we are assuming that the kinetics of the reaction scheme are known, all the kinetic constants in terms of along with the order of the stoichiometric coefficients as here, along with that we need we already know the order of each reaction and then the constants involved in the rate expressions all those things are known and they are part of the problems specification here.

So, if you are now looking at fluid flow, a single phase fluid flow in which consists of a mixture of all these species which are participating in this, then as the flow is taking place as heat transfer and mass transfer all those things are taking place there are the fundamental laws of mass conservation, momentum conservation, energy conservation, equation energy conservation and species conservation equation have to go and the corresponding laws are what we are going to write down here and we will start with the mixture mass conservation equation.

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And we are writing them down for a constant property fluid, we can always write down the more complicated form, but for our easy understanding we will take down the simplest form with constant properties of the fluid including the species. So, all the relations like thermal conductivity, specific heat and other properties of individual species kind of a mixture are expected to be known and constant when we are writing down this simplified form of equations, and here, if rho is the density of the mixture, which is expressible as sum of the densities of the individual species.

We can we can write down the mixture equation in this particular form, where rho is the density of the mixture mass density of the mixture and give us a mass velocity of the of the mixture and we also have the momentum conservation equation for the mixture is again dou rho by dou t. In fact, here rho is constant. So, we can cross this out and then you can take it out and that becomes del dot u equal to 0 and here we have dou u by dou t plus del dot uu, this is the dyadic velocity vector tensor is given by nu del square u plus g. So, we can write this also as dou u by dou t plus del dot del u plus g here. So, this is the momentum conservation equation and we have also forgotten the pressure gradient so that comes out here like this.

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Minus 1 by rho gradient of pressure, we now have the energy equation; energy conservation equation. This again can be different types of energy and we have finally, derived an expression for in terms of enthalpy from that assuming constant properties, we had an equation written in terms of temperature, here we have more terms. We have dou t by t with capital t is a temperature plus del dot ut and t is of course, a scalar whereas, u is vector here and del is the also a gradient operator it is a vector and that is equal to k by rho cp times del dot del t, we have just put the del square t as del dot del t plus mu by rho cp times phi v, this is all the rate of work done by the viscous forces and qr is the heat release because of the chemical reaction that happens in this divided by rho cp and in this equation we have neglected any contribution from gradient of heat transfer.

So, this is there is no radiative heat transfer involved in this if there is a radiative of heat transfer and if there is a flux of radiative heat coming from the surfaces of the control volume then that will also come as additional heat flux term through the control surfaces. So, this is the energy conservation equation and we also need to have a definition of density and all that. In fact, for a mixture we need to keep these things.

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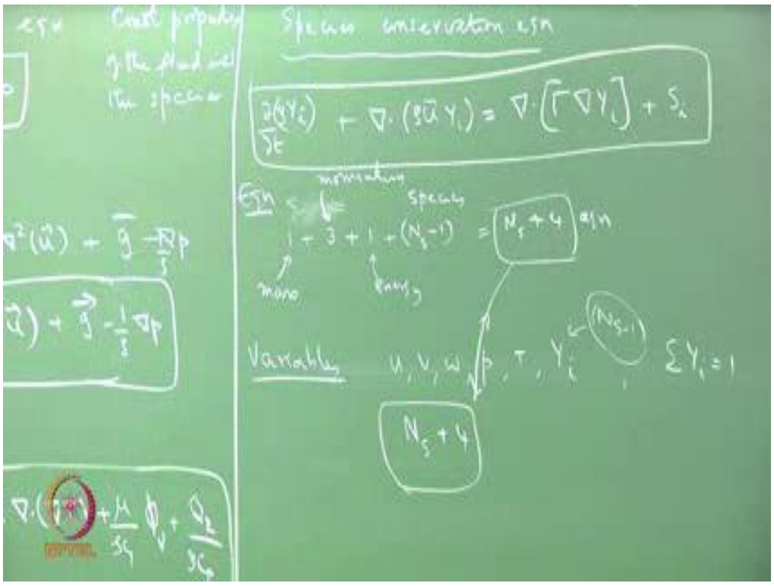

So, we need to have the species balance equation and this we have put in the form of the mass fraction of the species.

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So, we can we have put this in the form of species mass fraction yi as dou by dou t of rho yi plus del dot rho uyi equal to del dot gamma gradient of y plus s of i and what the subscript i here indicates is a species, for example, ya, yb, yc and so on or y auction or y carbon dioxide, y steam those type of things and so this is a mass fraction of the species and something come coming in and going out because of the flow and diffusing and s is essentially the rate of formation and we need to have an expression for the rate of formation of this species here. We need to have an expression for the rate of formation of this species here and similarly we need to have an expression for the rate of heat release because of the chemical reaction and both of these depend on the reaction mechanism here.

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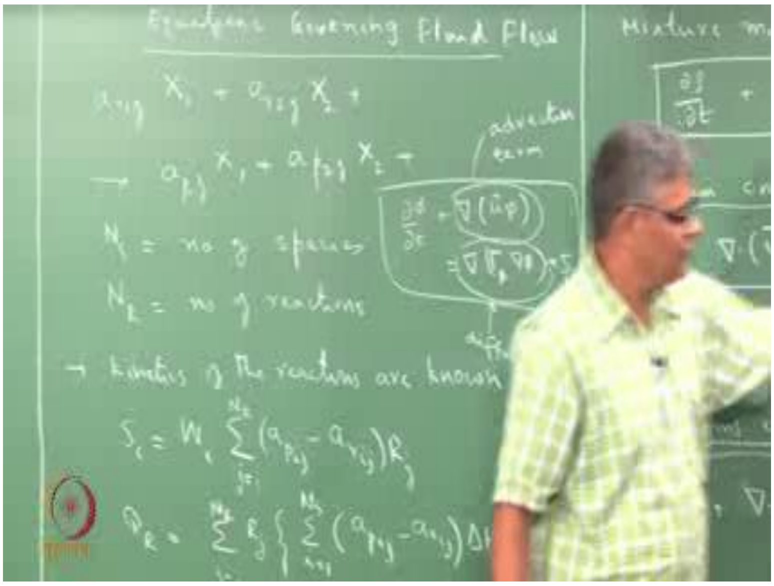

We can write down the values of the source term, which is going to appear in that in terms of the molecular weight and the individual rates of the reaction, which is given as so this is the rate of reaction of the jth reaction and in this reaction the ith reactant is appearing as a reactant with this stoichiometric coefficient in the jth reaction and therefore, it is disappearing at this rate, and it may also be appearing as a product with the coefficient of a pij. So, in which case it is being formed so that is an addition and the rate of formation is given by the rate of that particular reaction and the stoichiometric coefficient here and in a general case you have either this or this as non-zero or both as 0. So, it is unusual to have both being non-zero in the same reaction.

So, when it appears as a reactant the source term is negative and when it appears as a product the source term is positive, and the rate at which it happens is given by the stoichiometric coefficient of participation as a reactant or as a product times the rate of reaction and this can happen in any or all of the j reaction. So, we have to sum over all the reactions, all the j number of reactions in order to find out the total rate of formation of this and here these are in terms of stoichiometric coefficients.

So, we need to get that into multiply by the molecular weight of this species in order to get the source rate of formation here and similarly the heat release is expressed in terms of; this is sum over all the reactions sum of the product of the rate of reaction and so what we have here is in a particular jth reaction, ith species is being formed. So, you have that delta h heat of formation of the ith species and it may be disappearing because it is being consumed as a reactant here. So, that is minus here and it may be appearing as a product in which case it is a plus. So, whenever it is product of is formed then this heat of formation becomes positive quantity.

So, this happens for all the species, this has to be summed over all the species that are participating in this reaction and times the rate of that particular reaction and that is summed over all the reactions here will give us the total heat of this system of reactions. So, we have these rates of reaction and the heat of reaction terms which appear in the energy balance equation and the species balance equation. So, we have to be careful about the units and I leave it as an exercise for you to see that; see give the correct units for qr and si every equation of this has to be dimensionally consistent.

So, that is the sum total of these units of this particular term must be same as the units of this term and similarly the units of this and this and all those things must be the same. So, now, these are the 4 equations that we have put in blocks here are the equations that govern the flow of this reacting fluid containing ns number of species, which are reacting as per this nr number of reaction scheme which is given by the reaction scheme here and the rates of the reaction.

Now, how many equations are there? We have a total of 1 continuity equation plus 3 momentum equations plus 1 energy equation plus ns minus 1 number of species balance equations. So, this is species, this is energy and this is momentum and mass balance. So, that is ns plus 4 equations are there and what are the variables. So, these are the equations, we have the mixture u, v, w, the mixture pressure, the mixture temperature and the mass reactions of the species and there are ns number of species. So, we have this ns number of species, but we know that in addition to this we have sigma yi equal to 1. So, we need to know only ns minus 1 number of these to get the last 1 here. So, we have ns minus 1 number here plus 5. So, the total number of unknowns is ns plus 4. So, this total number of unknowns is ns plus 4 and the number of equations that are available is also ns plus 4. So, these 2 are the same.

So, we have these 4 equations plus the condition since we have put the species balance equation in terms of the mass fraction all the species will have to add up to a total of 1 is an extra algebraic constant that is coming out and because of that we need to know only ns minus 1 number of yis and the last one, the remaining one is known from this equation. So, here we have, many number of equations in the simplest case of no chemical reaction and a single component fluid like that then the same equations apply here this becomes redundant and rho becomes the density of the fluid and nu becomes the viscosity here and in this equation qr will be 0, but all the other terms will remain.

So, you can have qr becomes 0 and si becomes 0 and yi is equal to 1. So, it is nothing, it is essentially the same as this 1 here because if yi equal to 1 gradient of 1 is 0. So, this term is 0 and here this becomes this and this becomes this. So, the species conservation equation reduces to the mass conservation equation which is not surprising and you have the other equations remain the same except for the heat of reaction which appears in the energy equation.

So, when you look at these equations these equations have a characteristic form, which is both advantageous for us and it is also something that we have to take note of when we attempt a solution of this and that characteristic form is what is essentially known as the transport equation form where something is written in terms of dou phi by dou t plus del dot u phi equal to del dot gamma phi times gradient of phi plus source term here. So, this is the standard form of this equation the rate of variation with respect to time of phi at a particular point xyz within the whole domain or within the fluid continuum is given in terms of; what is a term, which is known as the advection term here, the change in a particular at a particular point may arise because of the convective nature of the flow because of the flow because fluid velocities the quantity phi may change. This is known as the advection.

So, that is the net difference between what is being taken out and what is being brought in into your control volume and that is the advection term. So, associated with the flow of the particular fluid and this is the diffusion term, counter gradient diffusion is what is actually bringing in either momentum here and heat and also the mass transfer here that may be happening and so this is the diffusion of phi because of gradients of phi within the fluid continuum is what is causing this and this is a source term and this source term takes different forms, for example, here in the momentum balance equation pressure gradient is a source term and gravitational external force is a source term.

In the case of energy equation, energy conservation equation the viscous dissipation term here is a source term which will be leading to increase in temperature because of the flow, because of the work done again viscosity, if you have an exothermic reaction than that heat of the reaction may be a source term and in the species conservation equation, the rate of formation of the species is a source term. It can also be a second term if it is negative. So, these all these equations can be put in this particular form variation of a quantity is expressed in terms of the advection term, diffusion term and a source term with a corresponding velocity which is nothing, but the fluid velocity a diffusivity which varies in the case of in this particular case with return, when phi is equal to u here this is the kinematic viscosity and phi for the energy equation is k by rho cp and here it is the diffusivity with proper dimensions and the source term for phi can also be different for different equations for the continuity equation it is 0 and here it is as mentioned the gravity term and the pressure gradient and these things like this.

So, this is a general form of the equation and this particular form has 2 important contributions; one is the advection which means that it is directional and it is associated with the flow direction and diffusion which happens in all directions. So, part of it is directional and part of it is essentially a directional it is all directions not necessarily the same if it is isotropic then it is the diffusivity is same in all directions sometimes it is not necessarily isotropic, in which case this can happen more in a certain direction and less in a certain direction as a result of both these process you have a variation of phi within our domain x, y, z as a function of time will be changing as per this equation.

So, in the next lecture, we will be looking at having looked at all this partial differential equations which govern the fluid, we look at what are the appropriate boundary conditions given this specific nature of the governing equations which is where the quantity that is of interest is governed partly by directional terms like advection and a directional terms like the diffusion term and source term can be different they can be independent of the parameter phi that we are looking at or in some cases they can also be functions of the parameter.

So, we are looking at the boundary conditions and the initial conditions that are required to complete the mathematical formulation of the problem just the governing equations are not sufficient along with that we need to have the boundary conditions. So, we will discuss the boundary conditions and initial conditions which are necessary for us to have a well posed problem that is a problem, which has a potentially unique solution and it is the unique solution that we wish to find through a numerical solution. So, that would complete the next this particular module and we will deal this with this in the next class.

Thank you.