Computational Fluid Dynamics

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Module No. # 06

Dealing with complexity of physics of flow

Lecture No. # 33

Topics

Derivation of the series conservation equation

Dealing with chemical reactions

So, we know how to do the energy equation. Let us now deal with the other two aspects that are of interest of many cross applications. We are dealing, first of all, with mass transfer; for example, in the case of a drying operation or in the case of dissolution of one substance in another or in absorption of gases, and so many applications which can be there in which mass transfer is one of the process of interest; and the mass transfer is definitely influenced by the way the reactants affect and so on.

There is yet another application, which is of real practical importance. And this is the case where the reactants are not only exchanging heat and mass and momentum, but they also inter-reacting with each other, in the form of a chemical reaction, and then, new species are formed. And we would like to see, for example, how much of conversion is taking place of the reactants into useful products and even undesirable products, and how these can be controlled by controlling parameters like the temperature, heat flux, velocities and so on.

In such cases, we have to deal with the case of a number of species, number of species which constitute together a fluid. So, we can consider a fluid no longer to be to be that of a single component, but to be a mixture of several species; and the particular species is can be indicated by the subscript, for example, i or a b c like that.

So, in such a case, how do we how do we take account of the presence of the species and how do you account for mass transfer and how do we account for the chemical reaction. This can be done by trying to generate a species mass conservation equation. And the way that we generate the species mass conservative equation, is very similar to what we have already done for momentum conservation and energy conservation. So, we take a controlled volume, and we say that, that control volume has a fluid, which has a fraction of a particular species i. And from that, we know what is the total mass of species which is contained within the control volume.

And we say that rate of change, rate of increase of mass of species within the control volume is again subject to, what is coming in, the rate at which the species is being brought in along with the flow, and the rate at which it is being taken out of the control volume along with the flow, and then the rate of diffusion of species, because mass transfer can take place. It can take place, when you have a concentration radient; there are other contributors also to the mass transfer.

And there is also another reason why which will affect the species conservation, which is the chemical reaction; as a result of which the species may be disappearing, it may be consumed in a particular chemical reaction or it may be produced in a chemical reaction; and it may have a number of these chemical reactions occurring together in a given fluid mixture. So, all these things will have to be considered, in arriving at the overall species conservation equation. So, we take the control volume and we write down the species conservation equation in words.

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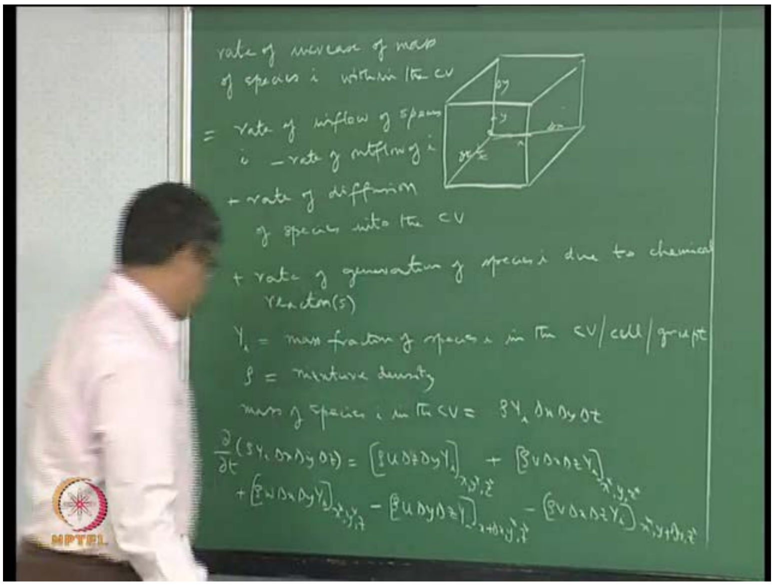

So, we start with trying to make a perfect control volume; hopefully we will get better and better time progresses, as the number of attempts become (()) and as usual we put our origin at the back bottom corner of this; this is our x direction, y direction, z direction, and we have delta x, delta y, delta z, as the three lengths of this rectangular parallelepiped, which is chosen in such a way that the faces coincide with the planes, which are along the coordinate directions. And we say that, this is our control volume, and we can say that, rate of increase of mass of species i within the control volume is equal to rate of influx, let us say inflow of species i, minus rate of outflow of species i plus rate of diffusion which is similar to, for example, the heat flux which is arising out of thermal conductivity and diffusion.

So, we have rate of diffusion of species i into the control volume plus rate of generation of species i due to chemical reaction. We have put chemical reaction, it can be a set of chemical reactions; so, we will put s in the brackets. So, this is a verbal statement and we can now convert it into a mathematical formula; we introduce a new variable, for example, y i, this indicates the mass fraction of species i in the control volume. in the control volume. Since this is our variable, this is also the variable that is defined at the grid point or at the center of the cell, so we can write as in the cell or at the grid point.

So, because it is a mass fraction, it has it is dimensionless; and rho is the overall density is the mixture density, then mass of species i in the control volume will be equal to rho y i times the volume delta x delta y delta z. So, from this, we can say that, y i is the mass density of the species I, per unit mass within that control volume. So, it is some sort of specific quantity representing the concentration of species, but we must note that, this is the mass fraction of species here. So, using this, we can we can write down the first expression as, dou by dou t of rho y I delta x delta y delta z and this is equal to rate of inflow of species.

Now, we are familiar with how to calculate the influx and out flux associated with the flow, and that is nothing but the mass flow rate through a particular face times the specific quantity per unit mass of that particular species. So, as mentioned here, y i is the specific quantity per unit mass of that particular species. So, we can say that, it is coming in through the left faces and the bottom faces and the back faces.

So, then the mass flow rate through the left face is rho u times delta x delta y times the specific quantity is y i; this whole thing evaluated at x y star z star; through the bottom face, the mass flow rate is rho v times, this is delta z, delta x delta z is the mass flow rate times the specific quantity y i, evaluated at x star y z star, where the starred quantities imply the centroid of that particular face. And similarly, the inflow through the back face will be rho w times the cross sectional area times delta x times delta y times y i at that particular point, that is x star y star z.

So, this is the inflow of species i, that is coming into rate at which the mass flow rate, mass rate which is coming into the control volume. And we have to subtract whatever that is being taken away by the fluid which is leaving the control volume; and the fluid is leaving the control volume at the right face, top face and the front face. So, we can evaluate again the mass flow rate rho u times delta y delta z times the specific quantity y i at that plane. So, this is x plus delta x y star z star.

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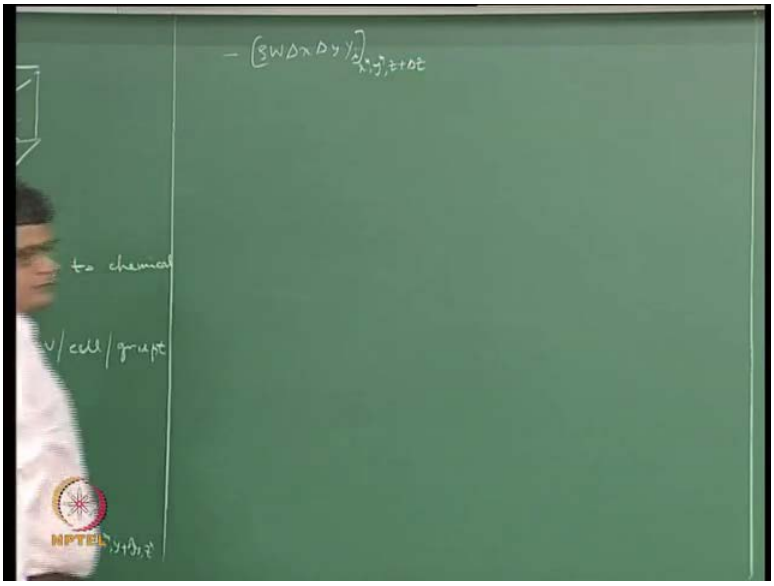

Through the top face, this is the mass flow rate, this is rho v times cross sectional area delta x delta z times specific quantity y i at x star y plus delta y z star. And we have through the front face, whatever that is leaving is the mass flow at rho w times cross sectional area delta x delta y times the specific quantity y i, at x star y star z plus delta z. So, these terms represent the rate of inflow and the rate of outflow; we have rate of diffusion, and what is this rate of diffusion?

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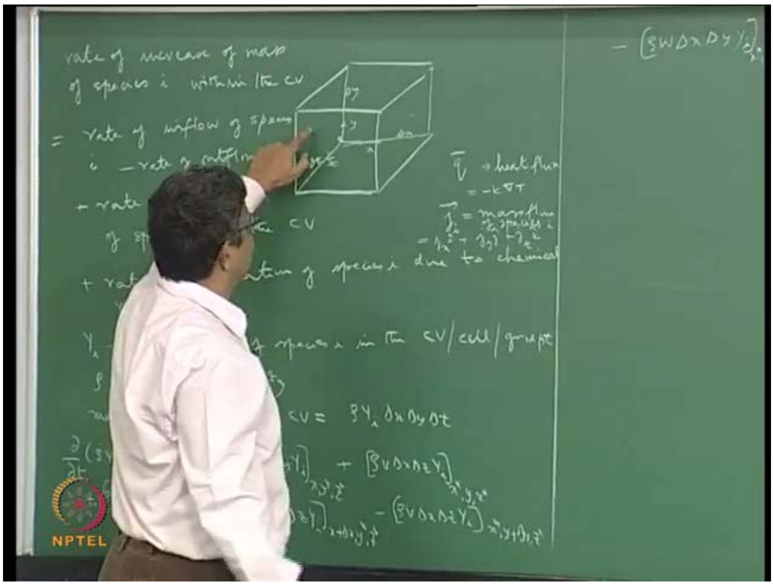

For the case of heat transfer, we have defined a heat flux vector and we invoked the fouriers law of heat transfusion to define this q as, minus k gradient of T, that is for the case of energy. And similarly, for the mass transfer which we know will take place, if there is a concentration gradient; just as a temperature gradient has given rise to a heat flux, a concentration gradient will also give rise to a mass flux and that will indicate as j. So, this j is a mass flux and this is a vector quantity. So, this has j x as the component in the x direction, j y in the j direction plus j z in the k th direction. So, this is the flux at, at any point in the three different components.

And the flux times the area normal vector; so, the j dotted with n is the actual flow flux that is coming in - the diffused flux that is coming in - or leaving the control volume. So, now, as defined before, j x is positive; when it is positive, it is coming, it is a flux in the x direction, because it is the x component. Similarly, if j y is positive, for example, 100, then it is the flux which is coming in the positive y direction. If we if it has to be negative, if it has to be flux in the negative y direction, this j y will be minus hundred. So, a positive quantity of j y implies that, flux is in the positive y direction; and similarly, positive quantity of j z implies, it is a flux in the positive z direction.

So, if we now consider the six faces of control volume, we can see that on the negative x face, that is on the left face, j x positive means, its acting it is coming in to the control volume. Similarly, on the bottom face, if j y is positive, it is coming into the control volume; and on the back face, j z positive means, it is coming into the control volume.

Similarly, on the right face, top face and the front face, j positive means, that it is a flux that is leaving the control volume; that means, it is a flux of species I, that is leaving the control volume. And we also note, that we have chosen the coordinate placed the surface of this control volume, such that, j dotted with n will have only one non zero component, for any surface. If we consider the left face here, then the outward normal vector of this particular plane is in the negative x direction, and it has no component in the y direction or the z direction.

So, that means that, the dot product of j dot n will have no contribution coming from j y and j z, because the surface area does not have any component. So, even though j y and j z are not zero at this point here, there is no flux coming into the control volume because of this, because we have an area vector which is perpendicular only to the x direction. And it has therefore no component with the y direction and the j direction. So, similarly, at the bottom face, actually the y component that comes in to the picture. So, keeping this in mind, just as we have done for the energy flux, we can now define the mass flux; and because we are talking about a specific species, we define j i as the mass flux of species i.

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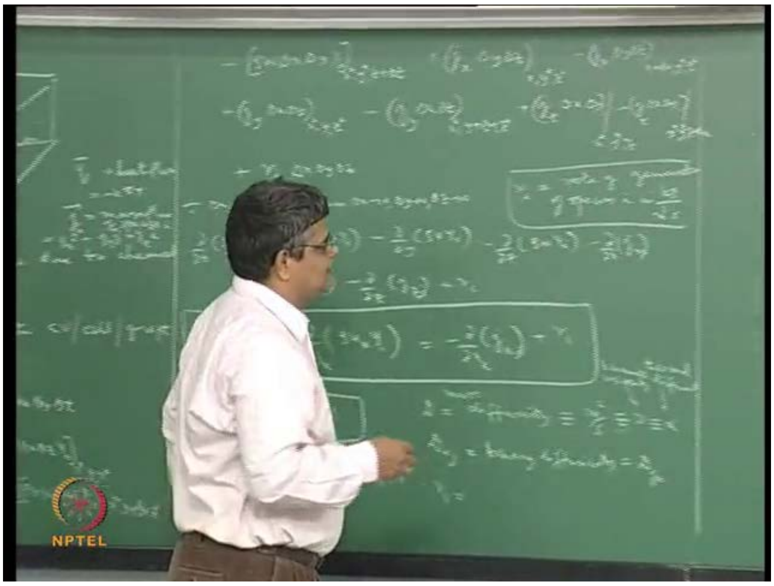

So, using this, we can now evaluate the flux that is coming in or through each of the faces. If you take the left face, then it is coming in. So, j x times the area delta y delta z is the total that is coming in, and this is evaluated at x y star z star. And if you consider the right face, then that is leaving, so minus j x times delta y delta z, at x plus delta x y star z star.

And the bottom face, it is only the j y component that is contributing and that is coming in, so, j y times delta x delta z at x star y z star through the top face, it is leaving. So, minus j y delta x delta z and this is at x star y plus delta y z star. And the back face, only the j z component will contribute, j z times the cross section area delta x delta y at x star y star z; through the front face, it is j z times delta x delta y at x star y star z plus delta z.

So, we have taken care of the rate of diffusion through the faces of the control volume, rate of generation of species i is there and we will just call it as r i. So, this is the rate of generation of the control volume and we have to get the units correctly to understand this. So, we are looking at, if you this equation must be consistent in terms of units, so every term in this must have the same units. y i here is fraction, so it does not have any units; this is kilogram per meter cubed times the volume is meter cubed. So, this whole thing is kilogram; so, it is kilogram per second.

So, r i here must represent the total generation rate, that is kilogram per second. What we will do is, we will we will multiply this by delta x delta y delta z. So, that now r i is the rate of generation of species i, in kilogram meter cubed per second. So, we will we will, for the time being, we will not specify what this is; once we derive the overall equation, we will look at how to specify the flux here and also the rate of generate term. So, this is the, now we have taken care of all the terms here.

As usual we will divide the whole equation by delta x delta y delta z, and take the limit as delta x tends to 0, delta y tends to 0, delta z tends to 0. If we do this, then we can see that the first term will give us dou by dou t of rho y i; and here if we take this term and the corresponding term at x plus delta x, this one these two together, then this will be rho u y i, at x minus rho u y i at x minus rho u y i x plus delta x at x minus rho u y i at x plus delta x divided by delta y in the limit at delta x tending to zero. So, these two together will give us minus dou by dou x of rho u y i.

Similarly, if we take this term, that is the flux coming through the bottom face at y, and the flux coming through the top face leaving through the top face here; these two will give us rho v y i at y minus rho u y i at y plus delta y divided by delta y, in the limit as delta y tending to 0, will give us minus dou by dou y of rho v y i. And the flux leaving through z face here and the z face here will obviously give us, dou by dou z of rho w y i.

Now, the fluxes here such that, if you divide these two by delta x delta y delta z, we get j x at x minus j x by x plus delta x divided by delta, in the limit as delta x tending to 0. So, that is minus dou by dou x of j x, and these two together through the bottom and top faces will give us minus dou by dou y of j y, and through the front face and the back face minus dou by dou z of j z plus r i. So, we have where r i is the rate of generation of species i per unit mass within the control volume.

So, as usual we can bring these minus terms to the left hand side, dou by dou t of rho y i, and we can write this in simple notation, dou by dou x k of rho u k y i; this is the advection term, and that is equal to minus dou x by dou x k of j k. We have to put the subscript i here to indicate that this is the flux of species i; so, this is k i plus r i.

So, this is the extra equation, which represents the change of species concentration y i in the control volume or at a particular point, and in so doing we have brought in a new variable y i; we have got a mass flux of species i to be specified. And the rate of production, rate of generation of species i from this to be, yet to be specified. As we have done in the case of heat flux, where we have said, where we have invoked the Fourier’s law of heat conduction here. We can also describe the mass flux arising through fixed law of diffusion; so, j i is minus d gradient of y i.

We have to be consistent here dimensionally. So, D here, we have to be very careful in this; we will see, this is the mass diffusivity. So, just as we have k as the thermal heat conductivity, and k by rho c p gives us the thermal diffusivity; and we have mu which is the dynamic viscosity, which expresses the relation between the sheer stress and the sheer rate. So, just similarly, and mu which is mu divided by rho, that is the momentum diffusivity. So, this mass diffusivity also has units of meter files per second, which is equal to nu, which is the kinematic viscosity; and the same as alpha, which is the thermal diffusivity. So, this is the kinematic viscosity and j here is kilogram; this whole thing here is kilogram meter cube per second here. So, this must be kilogram meter square per second. So, this is and we already have meter square per second here, and we have gradient; so, this is one. So, we should have rho here to make this consistent.

Let us just check. So, this is kilogram per meter cube times meter square per second and this is one by meter, because of this. So, this gives us kilogram meter square per second. So, this D here is the mass diffusivity, but generally it is not as straightforward diffusion; mass diffusion is not as simple as the heat flux here. When we have two species making up a control volume, then we call this as binary diffusivity.

So, if you have species i and j, then you call it as d i j; and d i j is the binary diffusivity, and it is defined in such a way that this is equal to d j i. And this binary diffusivity is a property of that particular mixture and it does not depend on the concentration of y i within that mixture. So, if you have two species y 1 and y 2, species one and two, then the binary diffusivity is not the function of y 1 and y 2; it is just a function of the two species which are interdiffusive; for example, if you take oxygen and carbon-di-oxide, they have a binary diffusivity which depends on the temperature and maybe pressure, but not on the concentration. But if you have a multicomponent mixture, so that is, when you have a fluid here is composed of more than more than two components, then this D here D i j is more than a diffusion coefficient; and that diffusion coefficient is much more difficult to determine than the binary diffusivity. And you will have contribution from large number of terms; it becomes much more complicated. And I would refer you to books in chemical engineering to get a better handle on this, on the mass diffusion term here, mass flux here arising out of this. So, as to bring out the similarity, we are just taking the case of two species, which are, which are constituting the whole mixture.

So, for more number of mixtures, we have to do much more work, before we can get this correctly. And we do not really have the time, but it is possible to do that, and it is the subject of transport phenomena and thermodynamics - thermodynamics of irreversible phenomenon and so on and so forth. So, let us not get too much in to, that the other thing that we would like to say is that, this is the mass flux. So, we have considered mass flux arising out of the concentration gradient of y, of species i. So, when there is a gradient, when between two point, if the species concentration is different, then there can be a mass flux as given by the diffusivity here.

Now, there can be other sources for mass flux; for example, because of temperature difference, temperature gradient, we can have mass flux, and that is known as the (()) effect. And then, you have other causes; because of the pressure differences, you have mass fluxes. So, those are typically small effect, similarly when we talk about heat flux, again we can have the Duffor effect, which brings in an energy flux term because of species variations.

So, when we talk about a multicomponent mixture, then the specification of the heat flux and the mass flux here become more complicated. If our flow problem really requires these various flux terms to be distinctly evaluated, then we have to consider those things. Otherwise, the predominant term which is contributing to the mass flux is the concentration gradient, and predominant term which is causing heat flux is the temperature gradient. So, we are considering only those things; otherwise, one would have to go through advanced books in transport phenomenon to consider this. And so, with this, we can say that, this is how we can specify the mass flux, which is coming in conservation equation. And so, when you put this inside, we see that we have an extra equation for y I, we have extra property, the binary b i for this the diffusivity can also be the same; for example, one species dominating the entire constitution of the mixture and if all the others are in trace quantities, then it is possible to choose a value of D i j, which is independent of the species concentration.

The other thing is that, when we add up all the species conservation equation, then we should get the overall good mixture conservation with the mass conservation equation.

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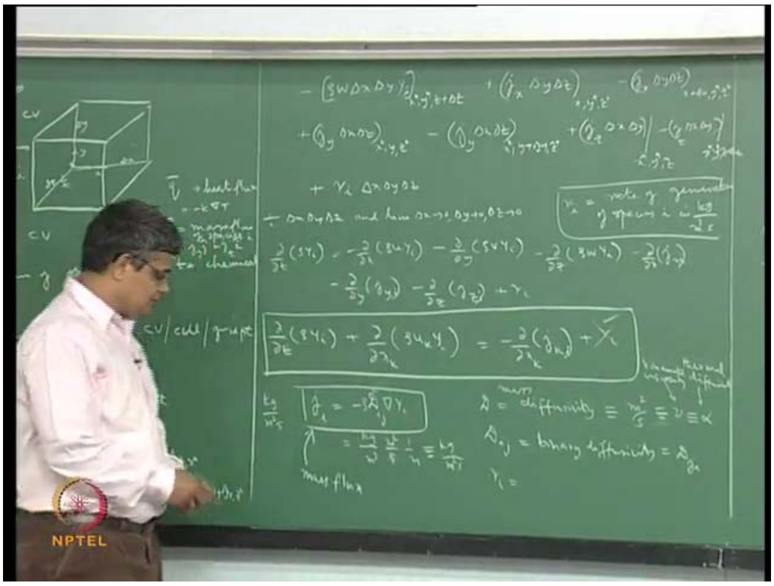

So, that puts specific constraints on the way, that the mass flux is actually defined. It puts constraints on the values of the D i j that can be taken now. So, this leaves us with the definition of what is r i. So, r i is the rate of generation of species, and the generation of species can be from a single reaction; and if you have multiple reactions, then each of the reaction will contribute to the generation, may contribute to the generation of species i. And typically this if you consider, for example, A plus B becoming C plus D as a standard chemical reaction, then for you have obviously four species here. So, you will have four species concentration equation and there is a rate of generation term associated with each of them. And for example, r A, that is rate of generation of species a, as per this reaction, it is actually not being generated, it is being consumed.

So, we will put it as minus a quantity. And if it is a homogenous reaction, that is, if all the four species that are in the same phase, then we normally write it as k some concentration of C times concentration of D, where C is concentration these can be related to the mass fraction; through the if you divide or multiply, where the using the molecular weight of species I, we can convert these things; and this is in the case of where k is the rate of reaction. And this rate of reaction is typically expressed as in terms of Arrhenius rate of reaction with pre-experiential factor, and an experiential term involving capital A, which is the activation energy and T is the temperature of the fluid in that at that particular point.

So, this is for an elementary reaction. And if this is not an elementary reaction, that is, if A and B molecules do not come together, but it goes through lot of intermediate transformations, then this rate of reaction may be dependent in different ways with the concentration; it is not linear as per this thing. So, these p and q define the order of the reaction - of the chemical reaction - and this information, all this information here, that is the p exponential factor, activation energy, the order for p and q, all these must be known and these come from the chemistry of the particular reaction; and these must be specified before we can evaluate this r A, which comes in to this (()) equation.

And you can have a series of reactions, for example, if you can have CH 4 plus o 2 giving rise to c o 2 plus H 2 o; you can balance this. And we can also have the c o 2 becoming c o plus o 2, as again this can be balanced. So, that you can have, when methane reacts with oxygen, then you can have partially depending on temperature and other things. You may have some amount of carbon monoxide produced and some amount of carbon dioxide produced. And depending on the conditions in which the reaction is occurring, the concentration of the c o as a product or c o 2 as a product may change.

So, in such a case, you have one reaction, one in which c o 2 is the product and reaction two in which case it is a reactant. And you can have reaction rate r 1 here, reaction rate k 1 here and k 2 here; and one has to evaluate the generation term and then the consumption rate from this, and then put together to evaluate the overall r i. So, that depends on the stochiometry and the rate expressions for this, in terms of pre exponential factor and activation energy and so on. So, the point that is being made here is that, if you have a sequence of reactions involving certain species and if the reaction rate for each for each of these is known, then it is possible to come up for each species - the overall rate of generation of that particular species. Taking account of its participation in all or some of these reactions either as a product or as a reactant, but the information of the chemical nature of the reaction, the chemical kinetics of this reaction, in which way they combine, as to which stochiometry they combine and at what rate the reaction rate progresses, what is the influence of various species concentrations on these, all this is to be determined is to be known. And if they are known, then they can be incorporated into this; and we should also consider, when we look at this r i here, we should distinguish between homogenous reaction and the heterogeneous reaction.

So, homogenous reaction is one which is taking place in the fluid, whether it is a liquid mixture or a gaseous mixture, heterogeneous reaction is something that is taking place at least between two phases; for example, if you take c plus o 2 becoming Co 2, c plus o 2 becoming c o - carbon monoxide and carbon dioxide - in which both carbon solid is getting combusted in order to produce c o 2 and c o. So, this is a solid, this is gas and this is gas. So, you have a reaction between a gas phase and a solid phase, and that is the heterogeneous reaction. So, the rate term here is only for the fluid part.

So, you have a rate term for this and a rate term for this thing, and these heterogeneous reactions usually come as boundary conditions; they do not appear in the rate of r i here and it is only the homogenous reaction which contribute to r i. So, we need to keep this in mind and we need to understand the chemistry of the reaction mechanism terms, in order to be able to compute r i appropriately making distinction between the homogenous reaction and heterogeneous reaction, and elementary reaction and non-elementary reaction, and the rate expressions involving the actual reaction rate and its dependence on the temperature and so on, and also dependence on the concentration of various species. So, once we have all these things, we have this term can be evaluated.

The flux term for simple case of two component mixture. So, it involves only binary diffusion, but for multi component system, it is much more complicated. People use Stefan Maxwell type of things to evaluate this, but this again can be expressed in the form of diffusivity or a diffusion coefficient, and the gradients of the species. So, together, these constitute the species conservation equation; for each species, if we solve this equation, we can get y i. So, that way, we are bringing in, in order to account for the chemical reaction, we are bringing an extra variable y i and extra information in the form of r i, which is dependent on the chemistry of the reaction. So, in a mixture of n species, you will have n equations like this representing y i. So, typically we will solve either n minus 1 species consideration equation or one overall mass consideration equation or we can solve n species equations.

So, for this particular case, for each species - additional species - that we want to bring in, we have to understand the diffusion term and then the reaction rate term, and then we can do it like this. For the specific case of pure diffusion and mass transfer without reaction, then this equation will work and we will just cross out this term, and this diffusive flux is given by the diffusions and so on.

So, for the case of simple mass transfer, it is only the first three terms that are present; with reaction, we have this. So, finally, we notice that this form of the equation, like the standard scalar equation, you have the temporal term, you have the advection term, you have the diffusion term and you have the source term. So, the inclusion of additional features like, heat transfer, mass transfer, chemical reactions, is not at all a problem in our c f d calculation, because it just adds, it brings in more equations of the same form. And since we know how to form a generic scalar transport equation, we can solve more number of these generic scalar transport equations, representing heat transfer, mass transfer with or without chemical reaction, along with the scalar transport equations, representing the x momentum, y momentum, z momentum and the overall continuity.

So, in this way, we can take account of more complicated cases, and we can extend c f d, which is computational fluid dynamics to c f t d or c f m d, where we have coupling temperature or energy equation with fluid dynamics, and mass transfer with fluid dynamics. All this is only for the case of laminar flows; we will see how we have to go beyond these equations to tackle the more difficult problem of turbine flow.