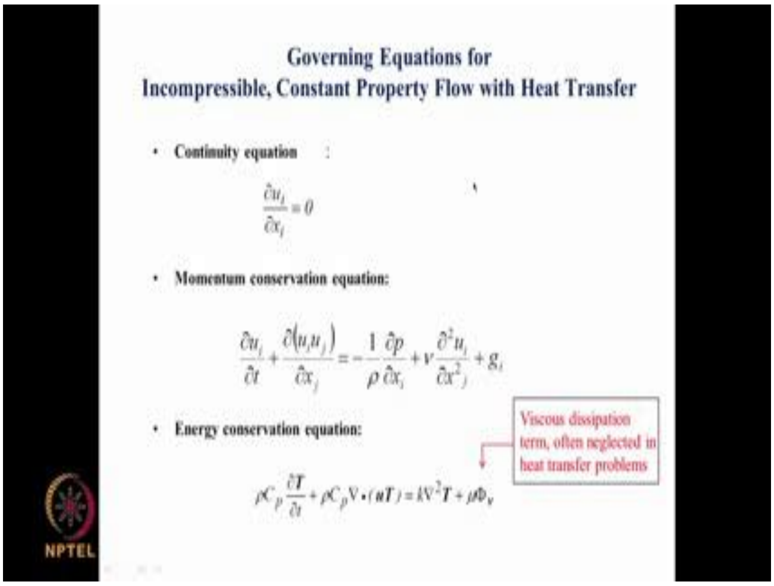
Computational Fluid Dynamics
Prof. Sreenivas Jayanti
Department of Computer Science and Engineering
Indian Institute of Technology, Madras

Lecture – 19
Practical cases of fluid flow with mass transfer in CFD point of view

In the last lecture, we have considered the case of heat transfer and we have looked at what kind of equations would represent a flow with heat transfer; that is, including the velocity, pressure and temperature. We derived a set of equations, which are summarized here.

(Refer Slide Time: 00:32)



Governing Equations for Incompressible, Constant Property Flow with Heat Transfer

- **Continuity equation** :

$$\frac{\partial u_i}{\partial x_i} = 0$$

- **Momentum conservation equation:**

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x^2_j} + g_i$$

- **Energy conservation equation:**

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \nabla \cdot (\mathbf{u} T) = k \nabla^2 T + \mu \Phi_v$$

Viscous dissipation term, often neglected in heat transfer problems

The governing equations for incompressible, constant property flow with heat transfer. We have a continuity equation, and a momentum conservation equation, the 3 momentum in the 3 directions; and then, we have an energy conservation equation, in which, through which, temperature is brought out as a free variable. So, the set of these 5 equations together, have as variables the 3 velocity components u, v, p, u, v, w, the pressure, and the temperature, as a set of 5 variables. And, the solution of all these things requires it in material properties which include the density, the viscosity, kinematic viscosity, thermal conductivity, and the specific heated constant pressure. So, with these things, it is possible to write down the set of governing equations.

(Refer Slide Time: 01:32)

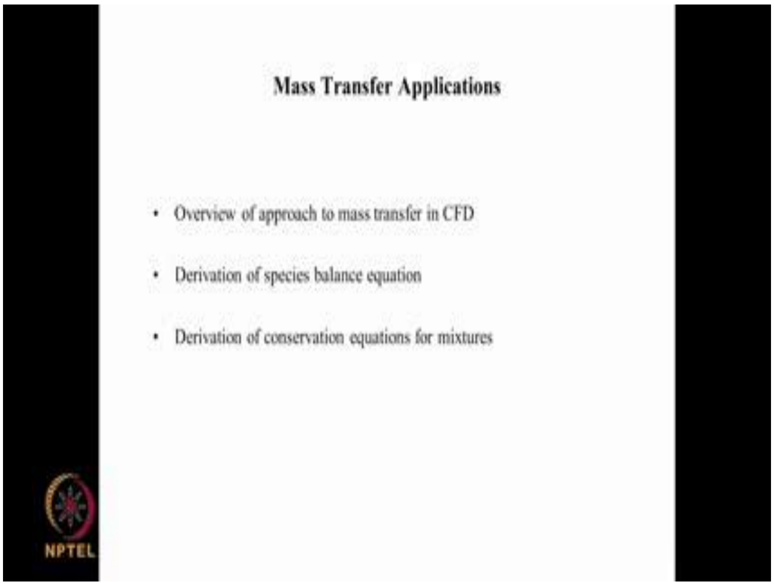
Heat Transfer Applications

- Convective heat transfer
- Conductive heat transfer
- Radiative heat transfer (**not in the syllabus for exams**)

And, we considered how these governing equations could represent the case of convective and conductive heat transfer that we know of, without having to specify any heat transfer coefficient. In the case of radiative heat transfer, of course, we have seen that, we need to do lot more work in order to get a proper description of radiative heat transfer, and that radiative heat transfer is not included in the set of equations which we have just now seen.

In today’s lecture, we are going to do something similar for mass transfer. If you have a flow with mass transfer, then, what are the equations that will describe this. So, we are going to look at mass transfer applications, and, we will try to structure it in a proper way, so as to understand it in the short amount of time that is available for us.

(Refer Slide Time: 02:13).



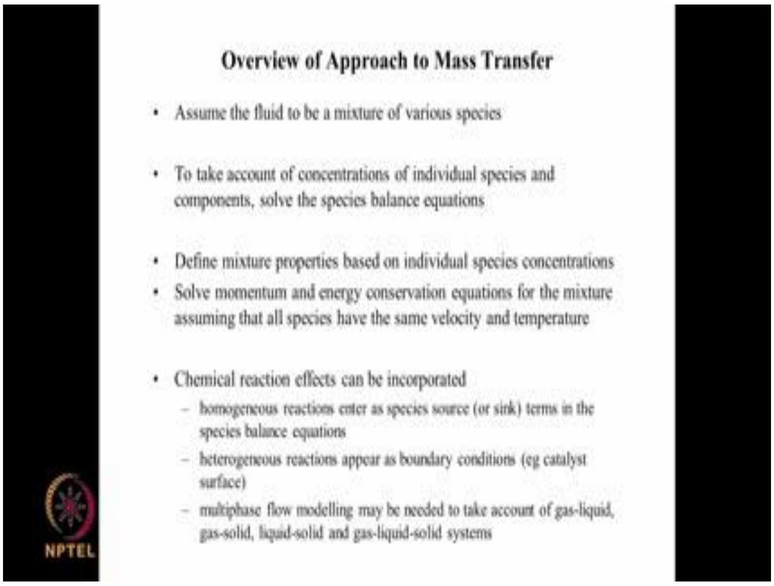
Mass Transfer Applications

- Overview of approach to mass transfer in CFD
- Derivation of species balance equation
- Derivation of conservation equations for mixtures

So, we are going to look at the overview. We will take an overview of the approach to mass transfer within the framework of CFD. We have seen that, within the framework of CFD, heat transfer requires, in a certain way, is treated, is done, in a certain way. So, how do we do mass transfer in this? And, as part of this, we will be deriving the species balance equation, a mass conservation equation of species. And then, we will also look, we will derive the conservation equations of momentum and energy for mixtures, because, mass transfer requires us to have at least 2 species, so that, one species is going from one part of the fluid domain into another part of the fluid domain, so that, there is mass transfer between, across gradients, and all that. That requires us to identify species. And so, we are considering the fluid now to be a mixture of different species, and the approach that we have in CFD is that, we have separately, species balance equations, and we have, also have a mixture balance equations.

So, those corresponding equations are what we are going to derive, in the rest of the lecture. The approach is given, summarized, in this slide.

(Refer Slide Time: 03:50)



Overview of Approach to Mass Transfer

- Assume the fluid to be a mixture of various species
- To take account of concentrations of individual species and components, solve the species balance equations
- Define mixture properties based on individual species concentrations
- Solve momentum and energy conservation equations for the mixture assuming that all species have the same velocity and temperature
- Chemical reaction effects can be incorporated
  - homogeneous reactions enter as species source (or sink) terms in the species balance equations
  - heterogeneous reactions appear as boundary conditions (eg catalyst surface)
  - multiphase flow modelling may be needed to take account of gas-liquid, gas-solid, liquid-solid and gas-liquid-solid systems

We assume the fluid to be a mixture of various species, and we take account of the concentration of individual species, and components. For this, we solve the balance equation, a species balance equation. And, we define mixture properties based on individual species concentrations. And, we solve the momentum and energy conservation equations for the mixture, rather than for the individual species. If you do that, then, we have too many variables, and it is not worth all the trouble. It is possible to make some simplifying assumptions, which can be restrictive in certain cases.

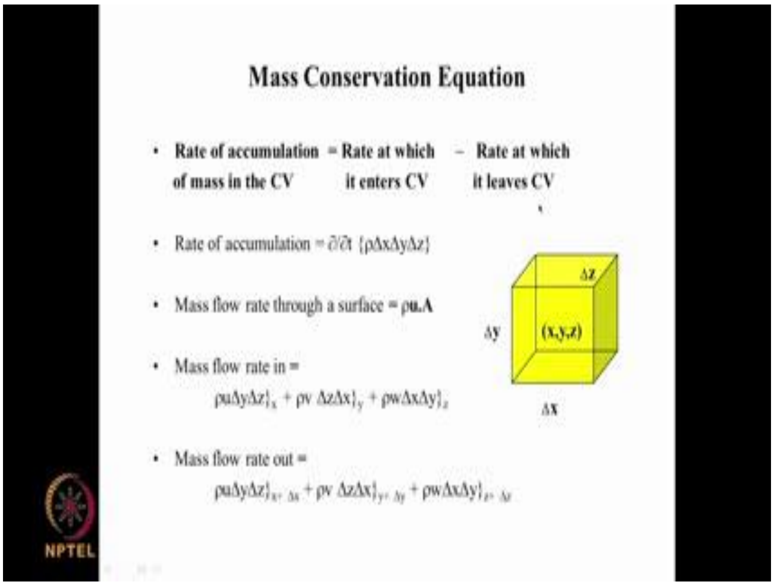
It is possible to make those kind of assumptions, and reduce the complexity of the problem, and bring it into a mixture momentum balance equation, and a mixture energy balance equation, but, a species mass balance equation. So, with this kind of formulation, it is possible to tackle mass transfer with, and without chemical reaction. And, the effect of the chemical reactions can be incorporated. In the case of homogenous reactions, these enter into the overall calculations scheme, in the form of, either a source term, or a sink term, of the species balance equation. So, there is a certain rate of generation, or rate of destruction of a species, because of chemical reactions. We are not considering nuclear reactions. Therefore, there is no destruction, or generation species from that. But, a chemical reaction can change the species, although the elementary balance always has to be satisfied.

So, what we are looking at is the species balance equation, and not the elemental balance equation, and that is something that we would like to highlight, as part of the derivation here. In the case of heterogeneous reactions involving 2 different species, heterogeneous reaction between a solid and a fluid phase is, obviously, coming as a boundary condition, because, we do not, we are looking at fluid mechanics.

So, the solid is a boundary, and so, any reaction between the solid and the fluid here, may come in as a boundary condition, in case, the solid species is on the walls of that particular fluid domain. If it is somewhere inside, finely dispersed, then, it may come as a, as a homogeneous source term. And, in the case of gas – liquid, or gas – solid, liquid – solid, gas – solid - liquid systems, which are finely dispersed throughout, where you do not have a clear separation of the domains, then, we have to do multiphase flow modeling, which is beyond the scope of this particular course. So, we are looking at, this is the overall approach.

So, when we want to deal with mass transfer, we have to do much more than the simple Navier Stokes equation. We need to have species balance equations; we need to have mixture balance equations; and, we need to have mixture momentum, and energy balance equations. And then, we need to have a framework for dealing with chemical reactions. So, we will do these things step by step.

(Refer Slide Time: 07:25)



Mass Conservation Equation

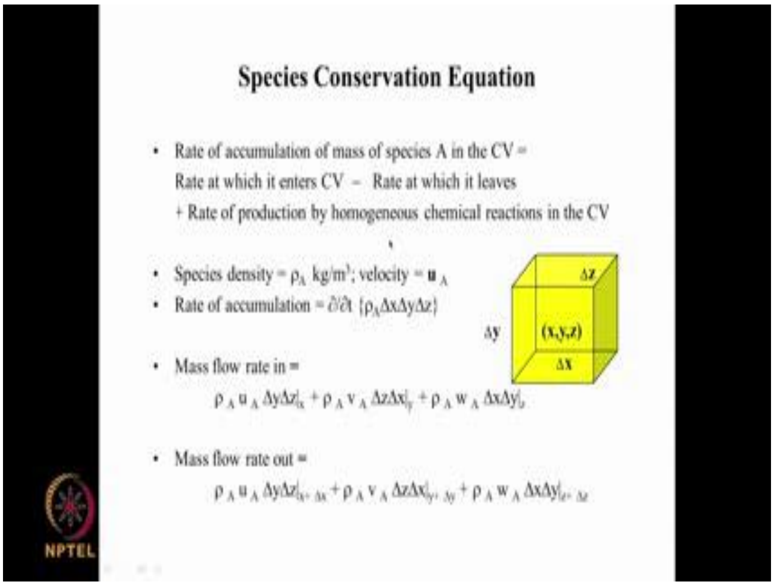
- **Rate of accumulation of mass in the CV = Rate at which it enters CV – Rate at which it leaves CV**
- Rate of accumulation = $\partial/\partial t\ \{\rho\Delta x\Delta y\Delta z\}$
- Mass flow rate through a surface = $\rho\mathbf{u}.\mathbf{A}$
- Mass flow rate in =

  $\rho u\Delta y\Delta z\}_x + \rho v\ \Delta z\Delta x\}_y + \rho w\Delta x\Delta y\}_z$
- Mass flow rate out =

  $\rho u\Delta y\Delta z\}_{x+\Delta x} + \rho v\ \Delta z\Delta x\}_{y+\Delta y} + \rho w\Delta x\Delta y\}_{z+\Delta z}$

So, we have already created a template for a conservation equation, for deriving the corresponding conservation equation. And, for example, for the mass conservation equation for a fluid, we considered a control volume, and then, we stated that, ‘the rate of accumulation mass within that control volume, in the absence of any, any sources, or sinks, is given by the difference between the rate at which it is entering, and the rate at which it is leaving here’. We can do something similar for a species conservation equation.

(Refer Slide Time: 08:00)



Species Conservation Equation

- Rate of accumulation of mass of species A in the CV = Rate at which it enters CV − Rate at which it leaves + Rate of production by homogeneous chemical reactions in the CV
- Species density = ρ_A kg/m^3; velocity = $\mathbf{u}_A$
- Rate of accumulation = $\partial/\partial t\ \{\rho_A \Delta x \Delta y \Delta z\}$
- Mass flow rate in =
  $\rho_A u_A \Delta y \Delta z|_x + \rho_A v_A \Delta z \Delta x|_y + \rho_A w_A \Delta x \Delta y|_z$
- Mass flow rate out =
  $\rho_A u_A \Delta y \Delta z|_{x+\Delta x} + \rho_A v_A \Delta z \Delta x|_{y+\Delta y} + \rho_A w_A \Delta x \Delta y|_{z+\Delta z}$

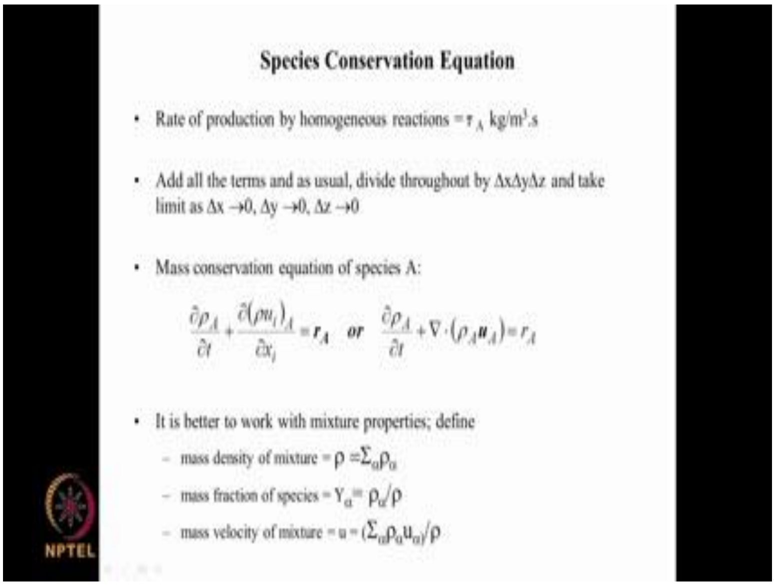
We take our magical cubical box, having delta x in the x direction, and having a height of delta y in the y direction, and a depth of delta z in the z direction here, with an origin which is located right there, which is xyz, so that, this point is x plus delta x by z; and this point is, x plus delta x, y plus delta y, z; and this point here is, x plus delta x, y plus delta y, z plus delta z. So, that way, we can identify all the 8 vertices of this box, and we can work with that. So, here, we are making a statement of the species conservation equation verbally, like, rate of accumulation of mass of species A in the CV, in the control volume, is equal to rate at which the species A enters the control volume, minus the rate at which it leaves the control volume, plus rate of production by homogeneous chemical reactions inside the control volume, ok.

So, we can consider that, throughout this, we note that, this particular volume, is in infinitesimal control volume in the fluid continuum, and we are saying that, this fluid continuum contains species A in a certain concentration. And, because of this concentration, and because of the presence of other species, species A can be either produced, or destroyed, used up, because of chemical reaction. And, this chemical reaction is happening in the, as a homogeneous chemical reaction; that is, in the same phase, either, within the liquid, or within the gas, within the fluid that we are considering here, and it is happening everywhere. So, that rate of production is what is considered here. In the case of destruction, this term will be negative. And, why we put plus here, because, in the absence of this rates at which it is entering, and this thing, production of the species will lead to accumulation. So, the left hand side is balanced by a positive value here, as a production term. So, rate of accumulation of mass of species A in the, in the CV, is equal to rate of production by chemical reaction, homogeneous chemical reaction in the CV, plus the net amount of species advected by the process of inflowing fluid, and outgoing fluid, ok.

So now, let us define, just like we have done for a fluid, let us define a species density rho A in terms of kilogram per meter cubed. And, we can also define a velocity u; here, it is a vector of species a. And therefore, we can consider the flow rate of species A through a particular phase can be rho A times u A dotted with the area vector of that particular surface. And, we also keep in mind that, we have chosen the surfaces of this cubical box to be aligned in the coordinate directions. So, with all those kind of, now, by now familiar things, we can write the rate of accumulation of species within the control volume as, the density times volume, which will give you the total mass of species A within the control volume. And, variation with respect to time, dou by dt of that, will give us rate of the accumulation of mass of species within the control volume, which is the left hand side of this. And then, the mass flow rate in, is what is coming in through the left phase, through the bottom phase, and through the back phase. And, in each case, we multiply rho times the velocity component perpendicular to that particular surface, times the area of that particular phase. For example, if you take the left phase, the area of that phase is delta y times delta z, and the density is rho A at x, and u A at x; because, this whole phase is located at x.

Similarly, through the back phase, the flow rate is given by w times the area of that particular phase. So, w a, the velocity of species a, the w component times the area delta x delta z, times rho A, here. And, all these things are evaluated at the midpoint of the corresponding phases. And, we note that, the variables may have different values at the midpoints of different phases. So, for example, rho A can be one value here, another value here, and another value at the back phase; another value at the bottom phase; all that. And similarly, u, v, w, can also change at every point within this, and specifically, at the centers of each of these phases. So, all the quantities here, all the variable values here, are always evaluated at the centers of the corresponding phases here. So, with that thing, we can, we can say that, we know how to evaluate the rate of accumulation term. We know how to evaluate the rate of entry, rate of inflow, and rate of outflow. Now, the rate of reaction, for the moment, we are calling it as r A, as per the chemical engineering practice.

(Refer Slide Time: 13:49)



Species Conservation Equation

- Rate of production by homogeneous reactions = r_A kg/m^3.s
- Add all the terms and as usual, divide throughout by $\Delta x\Delta y\Delta z$ and take limit as $\Delta x \rightarrow 0$, $\Delta y \rightarrow 0$, $\Delta z \rightarrow 0$
- Mass conservation equation of species A:

$$\frac{\partial \rho_A}{\partial t} + \frac{\partial (\rho u_i)_A}{\partial x_i} = \boldsymbol{r_A} \quad \boldsymbol{or} \quad \frac{\partial \rho_A}{\partial t} + \nabla \cdot (\rho_A \boldsymbol{u}_A) = r_A$$

- It is better to work with mixture properties; define
  - mass density of mixture = $\rho = \Sigma_\alpha \rho_\alpha$
  - mass fraction of species = $Y_\alpha = \rho_\alpha / \rho$
  - mass velocity of mixture = $u = (\Sigma_\alpha \rho_\alpha u_\alpha)/\rho$

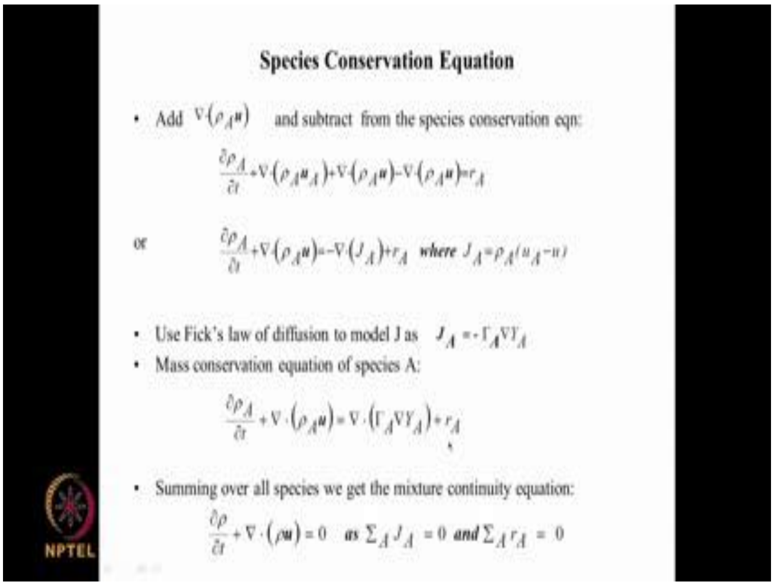
So, this is rate of production by homogeneous reaction. Why we are calling it as homogeneous reaction is that, this is a production term per meter cubed, and its kilogram per second per meter cubed, of this particular quantity of species A is being produced. And, if you multiply this by the volume, then, it will give you the kilograms per second. So, that is, rate of production of the species in the control volume. So, this is a volumetric generation term is what is mentioned here.

So, this is what will be coming out on, on this side here, because, this is rate of production, times the volume delta x delta y delta z, will give us the kilograms per second of production of species A in the entire control volume, and to that extent, we put this as a volumetric source term here. So, we add all the terms as usual, and then, divide by the product of the volume delta x delta y delta z, and take the limit as delta x tends to zero, delta y tends to zero, and delta z tends to zero. And then, we have an equation here, which is very similar to what we have for the mass conservation equation that we had earlier, except that, we have the subscript a denoting that, this is applicable for species A only. And, even the velocity components r for the species A only, and this is a summation over the three quantities, so that, you have dou by dou x of rho u, plus dou by dou y of rho v, plus dou by dou z of rho w; that is there. And, on the right hand side, we have the volumetric source term here. So, this can also be put in the vectorial form like this. So, this is very similar to the mass balance equation that we had earlier, but, in this particular case, this is only for a particular species of the entire mixture, and the species can be produced, or destroyed, by the, by a chemical reaction; and, to allow for that possibility, we are creating this rate of generation term here. In the absence of chemical reactions, this will be zero, and we will have just this. But, and, this is a species conservation equation.

We can go back, just like we have derived the mass conservation equation, we can also derive the species momentum conservation equation, and species energy conservation equation. So, if you do that, then, for each species, we will have a mass conservation equation, 3 momentum conservation equation, 1 energy conservation equation, like that. And, that becomes very tedious and very large set of equations, when you consider large number of species. And, number of species can be quite, quite high in certain cases; for example, in combustion, people are dealing with tens, and even hundreds of species. So, in that case, the number of equations becomes very complicated, complicatedly in large. So, what we would like to do is, to work with the entire continuum, and we, which is essentially a mixture of different species, and we define the mixture properties in the following way. So, the mass density of mixture rho is given by sum over all the phases, all the species, rho A, rho alpha. So, rho alpha is the mass density of species A, species alpha, and when summed over all the species, that will give us the density here.

So, now, you can define the mass reaction y of alpha, species alpha, is given by rho of alpha divided by rho. This is the mass fraction, and not the mole fraction. If you know the molecular weights, and all that thing, it is possible to come out with a mole fraction also. It is not a difficult thing to do. Right now, we do not need it. Similarly, the mass velocity of mixture which we are calling as u here, without any subscript; whereas, here, we have a subscript A; we have a subscript A here. So, without any subscript, we can define this as sum over all species of rho alpha u alpha, divided by the mass density, will give us the mass velocity. So, rho times u is the total flow rate, flux of that particular mixture, and, that is equal to sum of the individual fluxes. So, there is nothing complicated about it; it is pretty obvious definitions.

(Refer Slide Time: 18:57)



Species Conservation Equation

- Add $\nabla(\rho_A u)$ and subtract from the species conservation eqn:

$$\frac{\partial \rho_A}{\partial t}+\nabla(\rho_A u_A)+\nabla(\rho_A u)-\nabla(\rho_A u)=r_A$$

or $$\frac{\partial \rho_A}{\partial t}+\nabla(\rho_A u)=-\nabla(J_A)+r_A \quad \textit{where } J_A=\rho_A(u_A-u)$$

- Use Fick's law of diffusion to model J as $J_A=-\Gamma_A\nabla Y_A$
- Mass conservation equation of species A:

$$\frac{\partial \rho_A}{\partial t}+\nabla\cdot(\rho_A u)=\nabla\cdot(\Gamma_A\nabla Y_A)+r_A$$

- Summing over all species we get the mixture continuity equation:

$$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho u)=0 \quad \textit{as } \Sigma_A J_A=0 \textit{ and } \Sigma_A r_A=0$$

And, in order to get the, an expression which is more convenient, we do some algebraic manipulations, mathematical manipulations. So, we add this del dot rho A times u, where u here, is now the value of the mixture property, not of the individual property. And so, we have, this plus this equal to r A as the original equation. So, we add and subtract this quantity on both sides, and then, we can keep this here, and then, take it on to the other side, and we have del dot rho A u, and we have del dot rho A u A. So, we can write this thing as del dot rho A times u minus u A, when you take it to the right hand side.

So, this whole equation here, the original equation to which we have added and subtracted this thing, can be written in this particular form, where dou rho by, dou by dou t of rho A, plus del dot rho A times u, this is the mixture velocity, equal to minus del dot J A, this is the flux of that particular species, plus the rate of production term here. And, the flux here, J A is given as rho A times u A, minus u, which is a mixture velocity here. Now, this flux here, can be modeled using Fick’s Law of Diffusion, and so, this is given as minus diffusivity of A, times gradient of the mass fraction here. So, we have to be careful about the units of this. There are different ways of formulation of Ficks's law of diffusion, in terms of molecular mole fractions, and mass fractions, and all that. We have to make sure that, that definition is correct, and once you substitute this into this, we have an equation which involves rho by rho A, and all these things here. and so, this is the conservation equation for species a, and if you write down for all the species, and then, you add up all of them, then, for example, you get dou by dou t of rho A plus rho B plus rho C of all of them, and all the rho s summed up together will give you rho. And similarly, all of this will give us, give you rho here. So, you get this.

And, the formulation of the diffusive term, diffusive fluxes, and the production terms here, is such that, they will all add up to zero; because, if a is being consumed in a particular reaction, then, it is being, some other species is being, is produced. And, this is all happening within the control, within the liquid, the fluid continuum. So, there are some rates which are positive, and some rates are negative, for a different species. So, when you add up all of them, on a mass basis, this goes to zero. And similarly, sum over all the species of the diffusion thing, will also become zero, so that, we have, we recover the mixture continuity equation as this. So, we have a species balance equation, which is written in the form of involving the mass fraction of species, and if you divide this whole thing by rho here, you get rho A by A, which is Y A here. So, you have Y A here, and you have Y A here. And so, this whole species conservation equation can be represented in terms of a new variable, which is the mass fraction of species a. And, the rate of production of term is also divided by the mixture density; and so, that will give you the… This will be slightly different, ok.

(Refer Slide Time: 23:18)

Mixture Equations

- Species mass balance:

$$\frac{\partial \rho_A}{\partial t} + \nabla \cdot \left(\rho_A \mathbf{u}\right) = \nabla \cdot \left(\Gamma_A \nabla Y_A\right) + r_A$$

- Mixture continuity :

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \mathbf{u}\right) = 0$$

- Mixture momentum:

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \bullet (\mathbf{u}\mathbf{u}) = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g}$$

- Mixture energy with heat of reaction of Q_R:

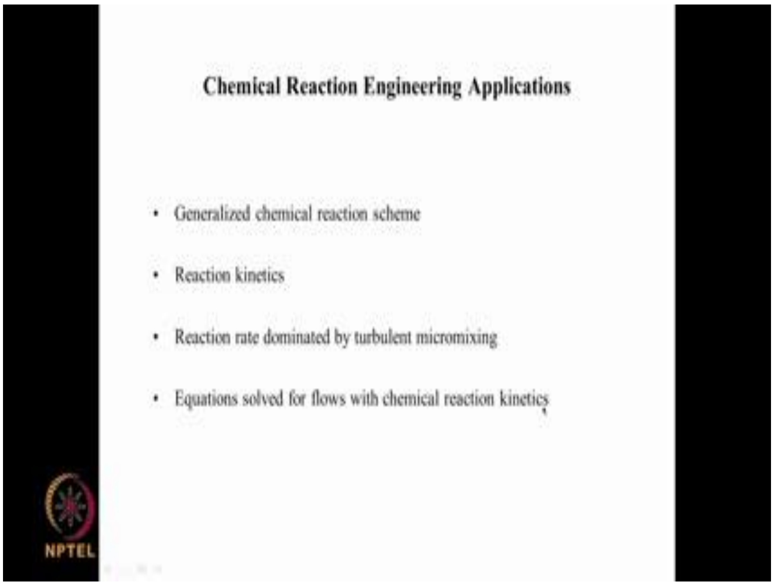
$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \nabla \bullet (\mathbf{u}T) = k\nabla^2 T + \mu \Phi_v + Q_R$$

So, the overall mixture equations can now be represented like this. Mixture continuity equation, mixture momentum equation will be very similar to what we have earlier; and then, mixture energy equation will have the usual term here, and then, the advection term, the conduction term, heat conduction term, the viscous dissipation term. But, there is also an extra term which is arising from the fact that, the reactions that are happening inside the liquid, inside the fluid continuum, can be, as a whole, they can be exothermic, or endothermic. So, depending on the progress of that particular reaction, there is a corresponding heat generation. So, this is the heat of reaction. This needs to be properly evaluated, and this becomes an extra equation, for our energy equation.

So, the mixture equations, to summarize, are, for every species, you have an extra equation here. So, if you have 3 species, you have 3 species balance equations. Now, when you add up all the 3 species balance equations, you get the mixture continuity equation. So, you either have 3 equations here, and no equation here, or you can have 2 species balance equation, and 1 mixture continuity equation. So, together, the species mass balance and mixture mass balance equations will constitute number of equations, which is equal to the total number of species. And then, we have 1 mixture momentum equation, which is like the same thing, except that, you know how mixture velocity and you have mixture density here, and mixture viscosity; and, those properties are based on the mass fractions, so, mole fractions of those individual species. And then, you have mixture density, mixture specific heat, and thermal conductivity here. And, together, we have an overall source term coming, which is essentially the heat of reaction of that particular, overall set of reaction scheme. So, this is the mixture equations, and in the case, in the absence of chemical reactions, this r A s and Q R s will be zero. And, if you have a mass transfer with dissolution, that dissolution is exothermic, endothermic, you can still have this. And, you can see a role for mass transfer. Mass transfer will change the mass fraction; you can have mass fraction gradients, and that is what is being resolved by solving this equation.

So, this scheme here can give rise to concentration gradients; can be used to evaluate concentration gradients. And, along with the concentration gradients, just as we have temperature gradients leading to heat transfer, convective, conductive heat transfer, you also have here, both the convective effect, and the conductive effect of the mass transfer is captured in this set of equations, through the introduction of a new variable, which is the mass fraction of the species. And, the number of additional equations depends on the number of species that are present. If there are N S numbers of species, the number of additional equations that come up is n s minus 1, because we already have the continuity equation that is accounted for. And then, we also have this Q R here. Now, we still need to specify what this rate of reaction is, ok.

(Refer Slide Time: 27:05)



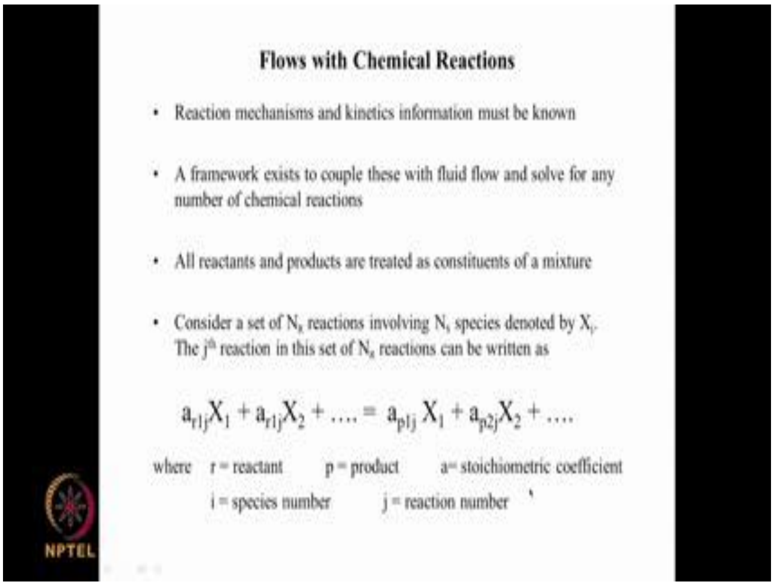
Chemical Reaction Engineering Applications

- Generalized chemical reaction scheme
- Reaction kinetics
- Reaction rate dominated by turbulent micromixing
- Equations solved for flows with chemical reaction kinetics

.

So, when we consider chemical reaction engineering applications, we need to have following additional things. We need to have a generalized chemical reaction scheme, the reaction kinetics, the reaction rate, which may be determines, in cases by turbulent micro-mixing, and other cases, by laminar diffusion of species. And, we will then look at the overall set of equations to be solved for flows with chemical reaction included, ok.

(Refer Slide Time: 27:41)



Flows with Chemical Reactions

- Reaction mechanisms and kinetics information must be known
- A framework exists to couple these with fluid flow and solve for any number of chemical reactions
- All reactants and products are treated as constituents of a mixture
- Consider a set of N_R reactions involving N_s species denoted by X_i. The j^{th} reaction in this set of N_R reactions can be written as

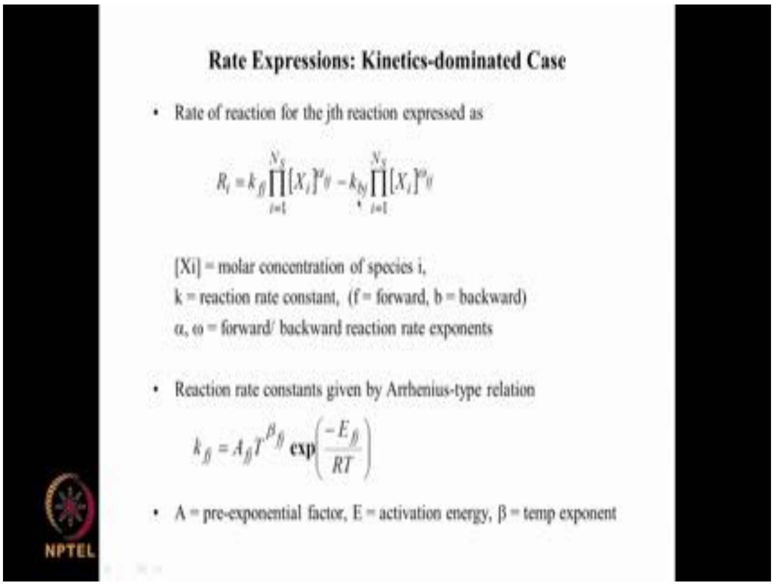
$$a_{r1j}X_1 + a_{r1j}X_2 + \ldots = a_{p1j}X_1 + a_{p2j}X_2 + \ldots$$

where r = reactant p = product a= stoichiometric coefficient
i = species number j = reaction number

So, when you are looking at flows with chemical reaction, the reaction mechanisms and kinetics of the information must be known. It is a part of the input. CFD cannot tell you what, what is a reaction mechanism. If you know the mechanism, then, it may say, because of the prevailing temperatures, this may be the rate of reaction, as per this Arrhenius rate of reaction, and all those kind of things. So, there is a framework that is needed to specify, and include all these reactions. So, there is a framework of calculation, which, that is present, and that we are going to see, which exists to couple this chemical reaction scheme with the fluid flow, and heat transfer, and mass transfer effects, all of which commit to the overall rate of reaction. And, this particular framework here, assumes that, we are dealing with the mixture. So, all reactions, and products, are treated as constituents of a mixture. And, consider a set of N R reactions involving N S species, denoted by X i here, and you have a stoichiometry of this each set, each reaction scheme within the set of reaction scheme is specified here. For example, you have species 1, and species 2, and all this species are participating with this stoichiometric coefficients in this reaction 1. So, you have a species number, and reaction number. So, and, you have reaction, on the reactant side here, and then, you have the product side. So, this is a typo here; this is reactant 2, r 2, ok.

So, you have j number of these equations, representing j reactions, which are, which are here. And, there are N S number of species, X 1, X 2, X N S, like this. It is not necessary that all the species participate in all the reactions, and it is not necessary that, there are certain reactants, and there are certain products. Sometimes, the same species may appear as a product, and sometimes it may appear as a, as a reactant; and this kind of a generalized scheme is what we start out with.

(Refer Slide Time: 30:07)



Rate Expressions: Kinetics-dominated Case

- Rate of reaction for the jth reaction expressed as

$$R_i = k_{fj}\prod_{i=1}^{N_S}[X_i]^{\alpha_{ij}} - k_{bj}\prod_{i=1}^{N_S}[X_i]^{\omega_{ij}}$$

[Xi] = molar concentration of species i,
k = reaction rate constant, (f = forward, b = backward)
α, ω = forward/ backward reaction rate exponents

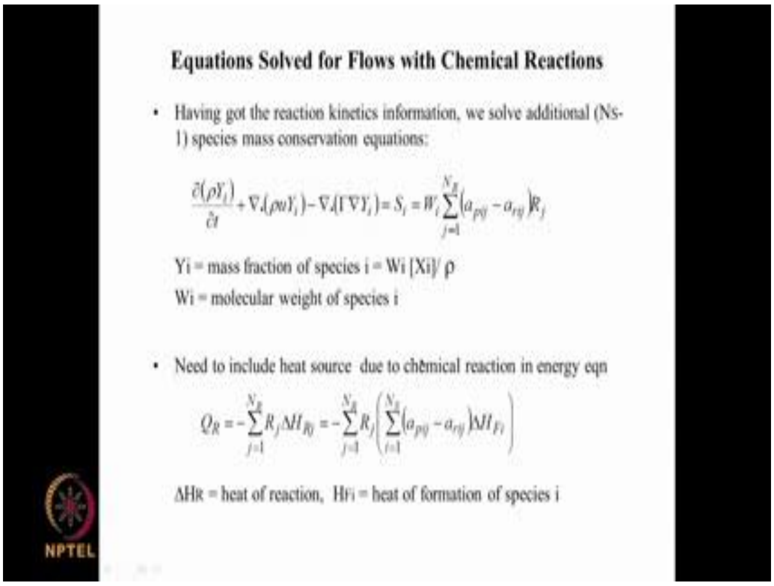
- Reaction rate constants given by Arrhenius-type relation

$$k_{fj} = A_{fj}T^{\beta_{fj}}\exp\left(\frac{-E_{fj}}{RT}\right)$$

- A = pre-exponential factor, E = activation energy, β = temp exponent

And, the rates of reactions of each of these are specified; for example, in the case of rate controlling reaction, in the form of a forward reaction rate, and a backward reaction rate, and concentration and exponents, here; so, expressing the order of the reaction. So, we can have, either this type of chemical kinetics controlled reaction, or, we can also have a turbulence dominated kind of thing, which we are not going to discuss here.

(Refer Slide Time: 30:36)



Equations Solved for Flows with Chemical Reactions

- Having got the reaction kinetics information, we solve additional (Ns-1) species mass conservation equations:

$$\frac{\partial(\rho Y_i)}{\partial t}+\nabla.(\rho u Y_i)-\nabla.(\Gamma\nabla Y_i)=S_i=W_i\sum_{j=1}^{N_R}(a_{pij}-a_{rij})R_j$$

Yi = mass fraction of species i = Wi [Xi]/ ρ
Wi = molecular weight of species i

- Need to include heat source due to chemical reaction in energy eqn

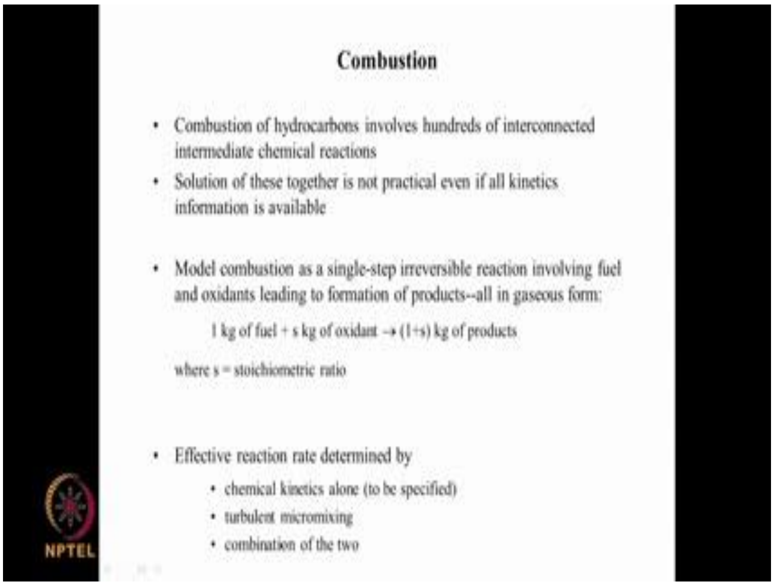
$$Q_R=-\sum_{j=1}^{N_R}R_j\Delta H_{Rj}=-\sum_{j=1}^{N_R}R_j\left(\sum_{i=1}^{N_s}(a_{pij}-a_{rij})\Delta H_{Fi}\right)$$

ΔHR = heat of reaction, HFi = heat of formation of species i

So, this is a general framework for expression of the reaction here, in terms of specified orders of the reaction, concentration of the reactants and products, and forward and backward reaction rates. And, these reaction rates are expressed in terms of a Arrhenius coefficients, in terms of activation energy, and then, temperature exponent and a pre-exponential factor.

All these things must be given. The entire reaction scheme must be known. The stoichiometric coefficients must be known. The orders of the reactions must be known, and the rate constants, the exponential factors, and all these things, must be known. If you know all these things, then, as part of the calculation scheme of the equations that we have already discussed, we know, at every point, what is the concentration of that particular species. So, then, we can substitute those things, and get the rate of reaction. And, from this rate of reaction, we can evaluate the overall heat source that is coming out, for each reaction, times the delta h of that heat of reaction of that particular reaction, and summed over all the reactions, will give us the total rate of heat generation, from set of all these reactions. So, having got the reaction kinetics information, we solve additional N S minus 1 species conservation equations. Here, we have expressed the species balance equations in terms of the mass fraction of species i here. The advection term, the diffusion term, and the source term, which is in terms of the molecular weights, and the reaction rates of the j th reaction, and the stoichiometric coefficients of the individual reactants species, as a reactant, and as a product. So, all these things will give us the overall species conservation equation. The momentum conservation equations, they do not change, except for the properties, which are now the functions of the concentrational species. And then, we have the source term in the energy balance equation; it is given in terms of the rates of the reaction, and the heat of the reaction, and the stoichiometric coefficients.

(Refer Slide Time: 33:12)



Combustion

- Combustion of hydrocarbons involves hundreds of interconnected intermediate chemical reactions
- Solution of these together is not practical even if all kinetics information is available

- Model combustion as a single-step irreversible reaction involving fuel and oxidants leading to formation of products--all in gaseous form:

  1 kg of fuel + s kg of oxidant → (1+s) kg of products

  where s = stoichiometric ratio

- Effective reaction rate determined by
  - chemical kinetics alone (to be specified)
  - turbulent micromixing
  - combination of the two

So, this completes the formulation for, as a kinetics control reaction, but if you have a, more practical cases like combustion are much more complicated; and simplistic treatment is done, where you have a fuel plus oxidant, giving rise to products, is a simplistic reaction scheme, in which the reaction rate is given (( )), sometimes by chemical kinetics alone, sometimes by turbulence alone, or may be as a combination of the two. So, that is beyond the scope of our course here, and we will, we can say that, we can look at a calculation framework, which is summarized in this slide, for flows with chemical reactions, in which we have a specialized form of the species balance equation N S minus 1 number of species balance equations; 1 overall continuity equation, 1 overall mixture momentum equation, the 3 in the 3 directions, and an overall energy equation, with an additional heat source expression coming here, from the reaction. So, in the next class, which will be in the form of a tutorial, we will try to write down these things on the board, and try to see exactly what these equations are. And then, try to put them in a common form, which we will then try, in the next module, to understand how to solve numerically.

Thank you.