Fundamentals of Combustion

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Lecture - 25

Governing Equations for Reacting Flow – Part 2 the Energy Equation

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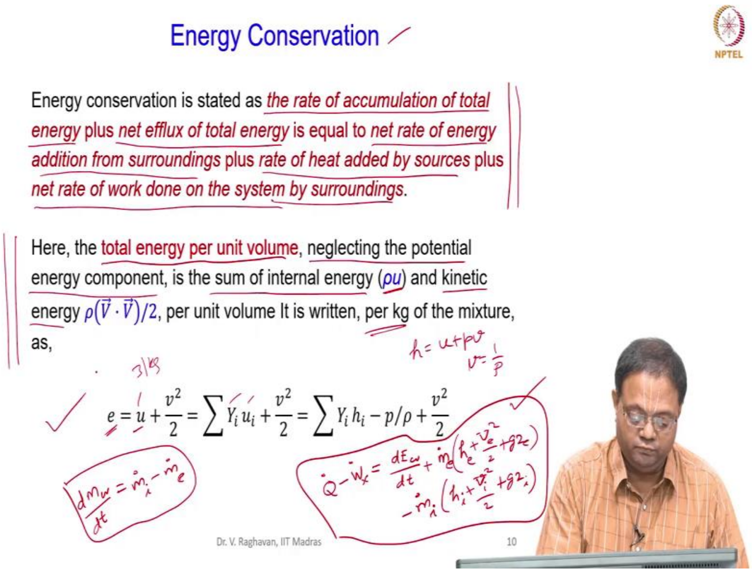

Energy Conservation

Energy conservation is stated as the rate of accumulation of total energy plus net efflux of total energy is equal to net rate of energy addition from surroundings plus rate of heat added by sources plus net rate of work done on the system by surroundings.

Here, the total energy per unit volume, neglecting the potential energy component, is the sum of internal energy (ρu) and kinetic energy $\rho(\vec{V}\cdot\vec{V})/2$, per unit volume It is written, per kg of the mixture, as,

J/kg

$h = u + pv$

$v = \frac{1}{\rho}$

$$e = u + \frac{v^2}{2} = \sum Y_i u_i + \frac{v^2}{2} = \sum Y_i h_i - p/\rho + \frac{v^2}{2}$$

$$\frac{dm_{cv}}{dt} = \dot{m}_i - \dot{m}_e$$

$$\dot{Q} - \dot{W}_x = \frac{dE_{cv}}{dt} + \dot{m}_e\left(h_e + \frac{v_e^2}{2} + gz_e\right) - \dot{m}_i\left(h_i + \frac{v_i^2}{2} + gz_i\right)$$

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So, energy conservation So, you know that if you have apply the first law for control volumes, you can write the energy conservation as the heat interaction between the control volume and the surroundings minus the work interactions.

$$e = u + \frac{v^2}{2} = \sum Y_i\, u_i + \frac{v^2}{2} = \sum Y_i\, h_i - p/\rho + \frac{v^2}{2}$$

Say, I am putting over head dot to indicate that the rate at which the heat is interacting and the rate at which the work is interacting. The suffix x here for the work is to indicate that this is the other type of work other than the displacement work which is which will not can happen in the control volume

So, that will be equal to the change of total energy within the control volume with time, the rate of change of total energy E_{cv}, capital E suffix cv is the total energy within the control volume as a function of time plus due to mass flow rates the energy will come in and go out, so the outgoing mass.

So, I will say outgoing mass is the mass which is exiting. So, $\dot{m}_e h_e$, its enthalpy plus the kinetic energy plus the potential energy of the outgoing stream. So, that minus what is coming in is $\dot{m}_i h_i$ plus the velocity $v_i^2/2$ plus potential energy, So, this is the overall conservation of energy in the control volume.

So, we can see that the rate at which heat is interacting minus the work done, by the control volume to the surroundings will be equal to the rate at which the total energy capital E changes with the time plus the mass which is leaving with its own enthalpy kinetic energy and potential energy minus the mass which is coming in.

So, the mass flow rate which is coming is $\dot{m}_i$. The mass flow rate which is going out is $\dot{m}_e$, h_i the enthalpy, $v_i^2/2$ plus gz_i that is the potential energy.

So, the mass conservation is written as the rate at which the mass within the control volume changes with time dm_{cv}/dt will be equal to, the mass which is coming in, the rate of mass flow into the control volume minus $\dot{m}_e$ which is the rate of mass flow out of the control volume. So, this is the mass conservation here and this is the energy conservation.

So, we can say that the rate of accumulation of total energy here, first term in the right hand side plus the net efflux of total energy that is this. Mass, with its own energy going out minus the mass with its own energy coming in this is the net flow rate of energy out of the control volume.

So, by dividing this by the area of cross section you get the flux. So, the net efflux the outgoing flux minus incoming flux of the total energy, is the total energy here, is equal to the net rate of energy addition from the surroundings it may be heat etcetera plus the net rate of heat added by sources that is within the control volume. There will be some sources which can generate heat plus the net rate of work done on the system or control volume by the surroundings.

So, these are the things you can add to this basically. So, this is the statement of energy conservation. Now, in thermodynamics point of view it is written in a simple manner like this. But when you want to write as a governing equation we should involve the partial derivatives and so on.

Now, let us go through one by one the terms. The total energy per unit volume, now for the practical situations the potential energies can be neglected easily.

So, the neglecting the potential energy component. Let us not take into account of that. So, what will be the total energy? That will be the sum of internal energy and the kinetic energy, per unit volume. Please see if you multiply this $\rho_u \times V$, so ρ density, into volume V that will be the mass into specific internal energy is small u, small letter u.

So, you can see that $\rho_u \times V$ (that will be the mass) × internal energy that will be the total internal energy. So, per unit volume it will be ρ_u. Similarly, kinetic energy $\rho V \times v^2/2$, that is the dot product of vectors, v .v/2, $\rho \times V/V$ its $\rho \dot{v}\dot{v}/2$. So, this is the total energy.

Now, we can write that in the specific form per unit kg, kg per unit mass of the mixture as e, the total specific energy will be equal to $u + v^2/2$. Now, u is actually what? J/kg.

So, now we can write this as a sum of mass fraction of each species $Y_i \times u_i + v^2/2$ and u, internal energy can be written by this definition of specific enthalpy h = u + pV.

So, using that I can write h as $Y_i h_i$ that is mass fraction of each species into its enthalpy – p/ρ. So, ν = 1/ρ, So, using that I can write this plus the kinetic energy $v^2/2$. So, this is the total energy component. So, let us see one by one the terms. So, this total energy changes within the control volume as a function of time, so that we have to conserve.

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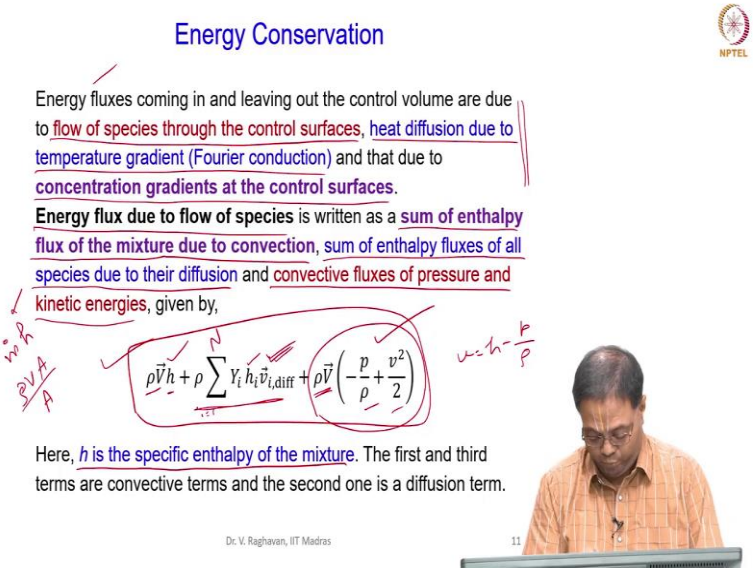

Energy Conservation

Energy fluxes coming in and leaving out the control volume are due to flow of species through the control surfaces, heat diffusion due to temperature gradient (Fourier conduction) and that due to **concentration gradients at the control surfaces**.

Energy flux due to flow of species is written as a **sum of enthalpy flux of the mixture due to convection**, sum of enthalpy fluxes of all species due to their diffusion and convective fluxes of pressure and kinetic energies, given by,

$$\rho\vec{V}h + \rho\sum_{i=1}^{N} Y_i h_i \vec{v}_{i,\mathrm{diff}} + \rho\vec{V}\left(-\frac{p}{\rho} + \frac{v^2}{2}\right)$$

$\dot{m}h$

$\rho VA/A$

$u = h - \frac{p}{\rho}$

Here, *h* is the specific enthalpy of the mixture. The first and third terms are convective terms and the second one is a diffusion term.

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Next is energy fluxes coming in and leaving out of the control volume are due to several things. The first one is the flow of species through the control surfaces. So, several species actually the mixture is crossing the control surface coming into the control volume through the control surface and again through a control surface its going out of the control volume.

So, this mixture consists of several species. So, we have to actually take into account of several species. So, flow of species through the control surfaces and heat diffusion due to temperature gradient. So, this is just Fourier conduction.

That is due to the temperature gradient there will be thermal energy transport that is the heat conduction that have to be taken into account. So, that is one of the energy fluxes. Then the concentration gradient at the control surfaces. Concentration gradients can prevail between the control surfaces due to which energy can be transferred.

$$\rho\vec{V}h + \rho\sum Y_i\, h_i \vec{v}_{i,\mathrm{diff}} + \rho\vec{V}\left(-\frac{p}{\rho} + \frac{v^2}{2}\right)$$

So, that is the energy fluxes 3 terms. Now, we have to expand each of these terms. So, energy flux due to flow of species that is nothing but this. 3 terms, first one is sum of enthalpy flux of the mixture due to convection.

So, there is a flow rate ρVA. So, ρVA is the mass flow rate. So, that is $\dot{m}$ into the energy which is transferred with this is h (enthalpy). For example, enthalpy is transferred. So, that term, sum of enthalpy flux.

So, this by unit area will give ρV. So, ρVh, the specific enthalpy that will be the first term that is sum of enthalpy flux of the mixture due to convection. So, something is coming in, some mass is coming in mixture mass is coming with its enthalpy mixture enthalpy h. So, this is the mixture enthalpy So, somehow mass is coming in and somehow this mass is going out. So, that we have to take into account.

Second is sum of enthalpy fluxes of all the species due to the diffusion. So, species this is by bulk convection the mixture is flowing with velocity of V. So, that by bulk convection mixture enthalpy is transported in and out through the control surfaces that is the first term.

Second term is diffusion individually a species can diffuse with their own species velocity $v_{i,diff}$. While doing so it will carry its own enthalpy h_i. So, ρY_i, the mass fraction of that ρ_i, density of the species rho $\rho \times Y_i \times h_i \times v_i$. So, this is diffusion due to the concentration gradient, thermal gradient and pressure gradient etcetera the diffusion velocity is calculated.

Predominantly, we can neglect the pressure gradient, surface body force gradient etcetera, but taking into account the ordinary diffusion at least we can calculate the diffusion velocity $v_{i,diff}$ and this into the mass of the species $\rho \times Y_i \times h$. So, you have to sum up for all the species. So, this summing up is i = 1 to n, for all n species this sum up is done. So, this is the total enthalpy flux due to the diffusion of the species. So, sum of enthalpy fluxes of all species due to the diffusion.

The first term is the mixture enthalpy that is convected by the bulk flow or the flow of the mixture itself. Second term is that, individual species are diffusing at their own rate diffusion velocity due to which the there is a enthalpy transport. So, that we have to sum up for all the species, 1 to n, if there are n species.

Then the convective fluxes of pressure and kinetic energies. So, that ρV into this energy. See for example, u has been written as h – p/ρ. So, that convection, is this term and last term together. So, the total energy is what u + $v^2/2$. So, that part will come as the third term, that is the convection of pressure and kinetic energies.

So, these are the 3 terms which will contribute to the energy flux due to flow of species. So, that is the first one. Then, second one here as I told you this h is the specific enthalpy of the mixture, and the first and third terms are the bulk mixture convection. The second term is diffusion due to each of species summed up.

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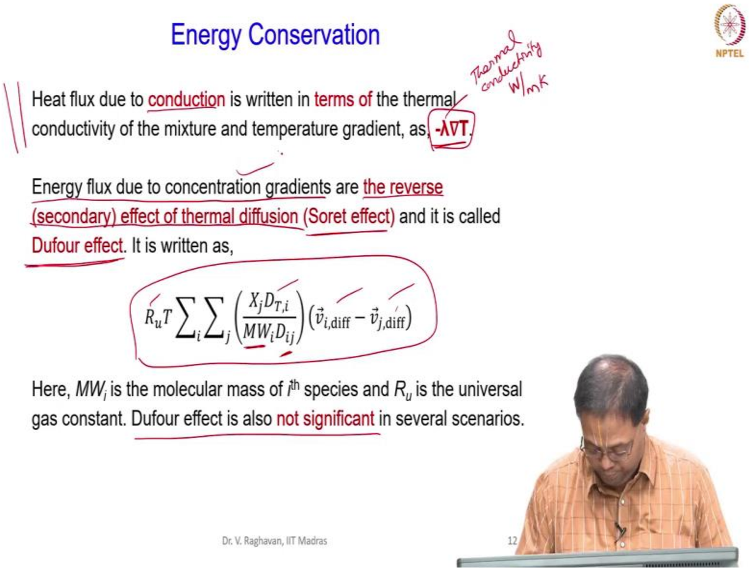

Energy Conservation

Thermal conductivity W/mK

Heat flux due to conduction is written in terms of the thermal conductivity of the mixture and temperature gradient, as $\boxed{-\lambda \nabla T}$.

Energy flux due to concentration gradients are the reverse (secondary) effect of thermal diffusion (Soret effect) and it is called Dufour effect. It is written as,

$$\boxed{R_u T \sum_i \sum_j \left(\frac{X_j D_{T,i}}{MW_i D_{ij}}\right)\left(\vec{v}_{i,\text{diff}} - \vec{v}_{j,\text{diff}}\right)}$$

Here, MW_i is the molecular mass of i^{th} species and R_u is the universal gas constant. Dufour effect is also not significant in several scenarios.

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Now, heat flux due to conduction, heat flux due to conduction, Fourier law. You have written in terms of thermal conductivity, the terminal conductivity of mixture and the temperature gradient. So, this is the term. Where λ is the thermal conductivity and the gradient of temperature.

So, you know that the negative sign appears because of the temperature decreasing from a particular point to another point and in the same direction the heat flow will occur.

So, heat flows in the direction of decreasing temperature. So, that is the flow, the heat flow depends upon the temperature gradient and if the thermal conductivity is higher the heat flow rate will also be higher. So, this is the heat flux term.

So, the previous term was the energy flux due to this species transport and second one is the temperature gradient the heat flux due to that. So, this is also a surface phenomenon. So, it enters into through a surface and leaves to another surface, the heat.

Then, the third term, the energy flux due to concentration gradients. Please understand that we have calculated the diffusion velocity correct, for any species as the sum of the diffusion velocity due to concentration gradient and due to the thermal gradient, soret effect.

So, now, this energy flux, due to the temperature gradient there is a diffusion of species. So, that again causes some concentration gradients. That will add energy to the control volume. So, that the reverse or the secondary effect of thermal diffusion, thermal diffusion is due to temperature gradient there is a diffusion of species from higher temperature to the lower temperature point that is termed as Soret effect

Now, the reverse of this, what happens is there is a contribution for energy flux due to the concentration gradient that is reverse effect called Dufour effect.

$$R_u T \sum_i \sum_j \left(\frac{X_j D_{T,i}}{MW_i D_{ij}} \right) (\vec{v}_{i,\mathrm{diff}} - \vec{v}_{j,\mathrm{diff}})$$

So, that is written as $R_u T$, and there is a summing up of this, mole fraction of here j into the thermal diffusion coefficient D_T of ith species divided by the molecular weight of i and D_{ij} is the binary mass diffusivity of any two species. We are summing up for i and j's.and the difference between the ith and jth species diffusion velocity. So, this is called Dufour flux, which is the addition of energy due to the concentration gradients. The reverse effect of the Soret effect. In the Soret effect what we saw was due to thermal temperature gradient species diffusion was happening, but here due to the concentration gradient energy flux is happening.

But in several cases this Dufour effect is not significant. So, we need not take into account of this. So, as I told you R_u is the universal gas constant and the MW_i is the molecular mass of the ith species. So, these are the 4 these terms. For example, here the energy flux due to flow of species is given as this. Then, the second one is the energy flux due to concentration gradients. Then, heat conduction, normal heat conduction is also added. So, these are the fluxes. So, these fluxes are nothing but the energy which is transferred through the control surfaces in and out of the control volume.

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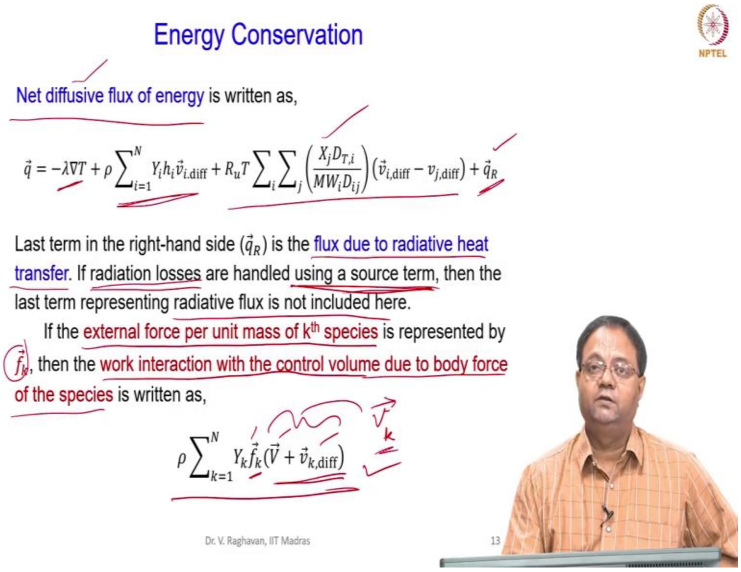

Energy Conservation

Net diffusive flux of energy is written as,

$$\vec{q} = -\lambda \nabla T + \rho \sum_{i=1}^{N} Y_i h_i \vec{v}_{i.\mathrm{diff}} + R_u T \sum_i \sum_j \left(\frac{X_j D_{T,i}}{MW_i D_{ij}} \right) (\vec{v}_{i,\mathrm{diff}} - v_{j,\mathrm{diff}}) + \vec{q}_R$$

Last term in the right-hand side ($\vec{q}_R$) is the flux due to radiative heat transfer. If radiation losses are handled using a source term, then the last term representing radiative flux is not included here.

If the external force per unit mass of kth species is represented by $\vec{f}_k$, then the work interaction with the control volume due to body force of the species is written as,

$$\rho \sum_{k=1}^{N} Y_k \vec{f}_k (\vec{V} + \vec{v}_{k,\mathrm{diff}})$$

$\vec{V}_k$

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So, now, we add up all the fluxes. Here, only the diffusion is taken into account. So, the thermal diffusion, then you can see this.

$$\vec{q} = -\lambda \nabla T + \rho \sum_{i=1}^{N} Y_i h_i \vec{v}_{i,\mathrm{diff}} + R_u T \sum_i \sum_j \left(\frac{X_j D_{T,i}}{MW_i D_{ij}} \right) (\vec{v}_{i,\mathrm{diff}} - v_{j,\mathrm{diff}}) + \vec{q}_R$$

So, please understand the diffusive fluxes I am adding up. So, heat conduction is also diffusion process, then the diffusion of enthalpy of each species summed up, that is one then Dufour effect. Dufour effect is the reverse of the Soret effect that plus you can also add that flux due to the radiative heat transfer.

There are two ways to handle radiation. One, we can assume that the radiation flux that is radiative energy per unit area enters through the control volumes and leaves through the control volume. So, there is a net radiative energy which is transported through the control surfaces into the control volume.

Now, we can also handle radiation losses or radiation heat transfer using a source term, volumetric source term. Then, you need not add this term here. So, the last term here is the flux due to radiative heat transfer.

Like conduction, radiation is also treated as a surface phenomena. So, through the particular surface, the radiative heat transfer per unit area enters and leaves to another surface and so on. So, the net energy which has come through the surfaces into the control volume can be calculated.

On the other hand, we can also take into account of the radiative heat transfer. Either may be losses or gain by the control volume. So, that predominantly flame actually loses its heat because of the high temperature area flame loses its heat to the surroundings.

So, I say radiation losses, that can be handled by source term. Source term means volumetric term. So, that will not come here in the fluxes. So, that is within the control volume it will add as a sink or source. So, that will be volumetric term that will be added. The last term representing radiative fluxes will not be included if the radiation losses are handled as a volumetric source term. That is the main point to note here. So here the diffusion fluxes are summed up like this. So, normally, this term can be neglected, the Dufour term can be neglected.

Now, let us take the body forces. The external force per unit mass of k^{th} species that is represented by $\vec{f}_k$, f suffix k vector. So, this is the term that is the external force per unit mass of the k^{th} species. It is some body force, some weight a particular species has. So, that will create some forces. So, that is the external force per unit mass of the k^{th} species. So, it is body force what we can call.

$$\rho \sum_{k=1}^{N} Y_k \vec{f}_k (\vec{V} + \vec{v}_{k,\text{diff}})$$

So, when you have such a representation the work interaction with the control volume due to body force of the species is written as the mass fraction of the species into body force of the species that is the external force per unit mass into the velocity of the species.

What is the velocity of species? The bulk velocity plus its diffusion velocity. So, this is nothing, but the velocity of the species k. So, now this $\rho \times Y_k$ will be the mass of this species into its velocity that will be the mass flux of the species into the body force. That will be the body force term. So, each and every species has its own body force, its weight basically. For example, carbon dioxide has a molecular weight of 44.

So, it may contribute to more external force than hydrogen, which has the molecular weight of 2. Now, this term is the external work, but this we have to add this to the work terms basically.

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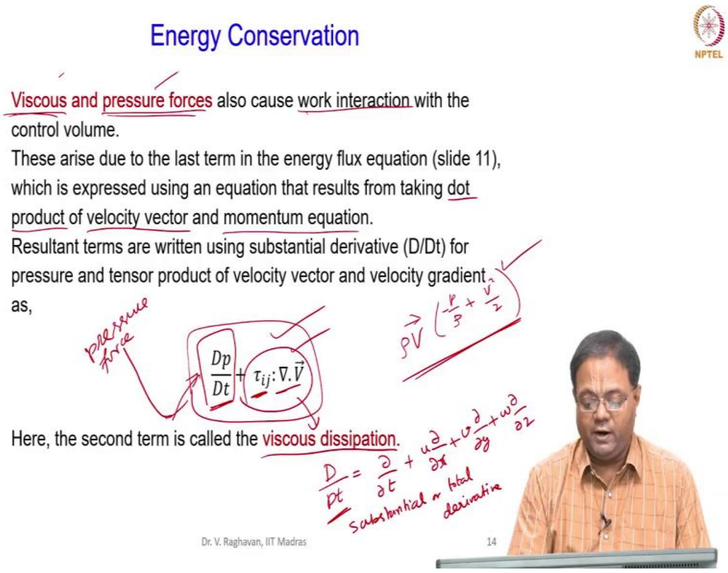

Energy Conservation

Viscous and pressure forces also cause work interaction with the control volume.

These arise due to the last term in the energy flux equation (slide 11), which is expressed using an equation that results from taking dot product of velocity vector and momentum equation.

Resultant terms are written using substantial derivative (D/Dt) for pressure and tensor product of velocity vector and velocity gradient as,

$$\frac{Dp}{Dt} + \tau_{ij} : \nabla . \vec{V}$$

Here, the second term is called the viscous dissipation.

pressure force

$\rho\vec{V}\left(-\frac{p}{\rho} + \frac{v^2}{2}\right)$

$\frac{D}{Dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z}$

substantial or total derivative

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Similarly, viscous and the pressure forces will also contribute to the work interaction w_x.

$$\frac{Dp}{Dt} + \tau_{ij} : \nabla . \vec{V}$$

So, let us see this slide number 11. Here, this term, this flux which is entering and leaving which is due to the pressure and kinetic energy, the pressure and kinetic energy that flux, $\rho V(-p/\rho + v^2/2)$. So, this is the kinetic energy and pressure energy.

This flux, if you take the dot product of this with the velocity vector and combine that with the momentum equation (derivation is not given here I am just explaining that due to this term you get the forces due to pressure and viscosity).

Body force is already taken into account. So work done due to pressure and the kinetic energy is derived like this. The substantial derivative of pressure that is Dp/Dt plus this is the stress tensor.

So, tensor product of the stress tensor and the gradient of velocity. So, this will give you the viscous forces. This term is called viscous dissipation term that is a force by the surroundings on the control volume. Similarly, this is the pressure force term.

So, this is the pressure force. Now, the substantial derivative D/Dt is written as the partial derivative with time plus convective derivatives. Convective derivative we can write the Cartesian coordinate as $u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z}$, where u, v, w are the components of velocity in x y and z direction. So, this is the substantial derivative or you can also say it is total derivative.

So, that total derivative of pressure will contribute to the work done by the pressure and the viscous terms are actually captured in the stress tensor, product of that with the gradient of velocity will give you the viscous dissipation term which is the work done due to the viscous forces.

So, these are the force terms. So, there are 3 force terms. Previously, in this slide we saw the body forces contributing to work interaction these force terms will contribute to work interaction basically.

So, external force per unit volume of each species added up with its mass and its mass flux basically which is this mass flux that is $\rho Y_k \times v_k$ that will be the mass of the kth species that into the body force of that will be the external force per unit volume of that unit mass.

So, $\vec{f}_k$ is the external force of the unit mass into the mass flux will give you the body force generated by the species k and that summed up for all the species will contribute the work interaction.

Similarly, the viscous and pressure force, this will cause work interaction. So, those terms are added here.

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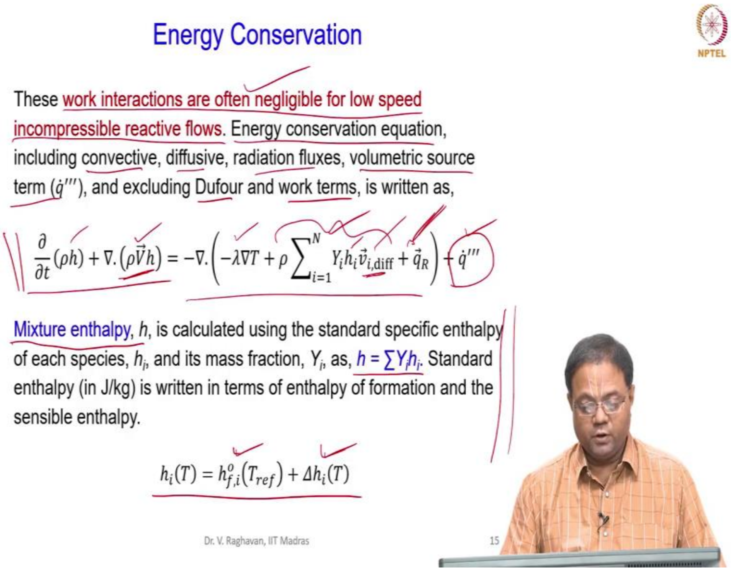

Energy Conservation

These work interactions are often negligible for low speed incompressible reactive flows. Energy conservation equation, including convective, diffusive, radiation fluxes, volumetric source term ($\dot{q}'''$), and excluding Dufour and work terms, is written as,

$$\frac{\partial}{\partial t}(\rho h) + \nabla.\left(\rho \vec{V} h\right) = -\nabla.\left(-\lambda \nabla T + \rho \sum_{i=1}^{N} Y_i h_i \vec{v}_{i,\mathrm{diff}} + \vec{q}_R\right) + \dot{q}'''$$

Mixture enthalpy, h, is calculated using the standard specific enthalpy of each species, h_i, and its mass fraction, Y_i, as, $h = \sum Y_i h_i$. Standard enthalpy (in J/kg) is written in terms of enthalpy of formation and the sensible enthalpy.

$$h_i(T) = h^o_{f,i}\left(T_{ref}\right) + \Delta h_i(T)$$

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So, next is, but for incompressible reactive flow low speed flows.

Only when the velocities are very high, pressure gradients are very high, then only the pressure forces, viscous forces and the body forces will be contributing to work interactions or else the work interactions are often negligible that you have to understand. So, all the terms have been explained now.

So, we will try to write the overall energy equation. So, energy conservation including convective term, diffusive term and radiation fluxes. So, I am adding the radiation either as a flux or a volumetric source, but in this case, I am adding as a flux from the control volume control surfaces it is coming into this and the volumetric source term this is this term etcetera.

$$\frac{\partial}{\partial t}(\rho h)+\nabla.\left(\rho\vec{V}h\right) = -\nabla.\left(-\lambda\nabla T+\rho\sum_{i=1}^{N}Y_i h_i \vec{v}_{i,\mathrm{diff}}+\vec{q}_R\right) + \dot{q}'''$$

But I am neglecting the Dufour effect and the work interaction terms, which I have explained how to write that, but we need not add if you want you can add it into this equation. For example, this is the work done due to pressure the substantial derivative of pressure and the viscous dissipation term. Similarly, this body force term, these 3 terms you can add it to the right hand side,

But I have not added because for low speed incompressible flows they are not significant. So, I have neglected that. So, other terms I have added and I am keeping the enthalpy conservation like this. So, the mixture enthalpy, the rate of change of the mixture enthalpy with time within the control volume plus the convective, this is the convective flux of the mixture enthalpy.

The convective flux is the outgoing mass flow rate into the enthalpy of mixture which is going out divided by the area that minus incoming. So, that efflux, is the second term convective term, it is a mixture velocity, mixture enthalpy and mixture density here. So, on the right hand side we have the diffusion fluxes. Diffusion fluxes, first one is the Fourier conduction and this term is the energy transport due to the diffusion species.

So, $v_{i,diff}$ is the diffusion velocity of each species, so rho $\rho Y_i \times v_i$. So, that is a diffusion flux of each species into enthalpy of the species i. That summed up for all the species that is the energy transported due to the diffusion of the species and here the energy transported due to radiation q, radiation through the control volume. So, I have taken this flux term and this is the source term, if there is any source that can be handled here. In some cases, it may not be used at all. So, the mixture enthalpy h is calculated using the standard specific enthalpy of species h_i or absolute enthalpy, h_i like this. See, for example h_i at any temperature T will be the heat of formation at the reference temperature of 298 K plus the sensible enthalpy which will take the temperature from T_{ref} to T.

$$h_i(T) = h^o_{f,i}\left(T_{ref}\right) + \Delta h_i(T)$$

So, the energy added due to that increase in temperature. This you have to find for all the species and this should be in mass basis, so that the mixture enthalpy can be calculated as the sum of product of mass fraction of each species into its specific enthalpy, mass based specific enthalpy. So, this you know. So, that is the total energy conservation.

So, you need the information of the species enthalpy of each species plus the mixture enthalpy. So, you have to calculate the thermal conductivity of the mixture, then you can see that here you are calculating the density of the mixture, and the enthalpy, then when you calculate the diffusion velocity you need the binary diffusion coefficient of all the species taken or the overall diffusion coefficient of the particular species going into mixture and so on.

Similarly, the heat transport due to the radiation can also be accounted here. So, this is the conservation of energy. You can see that additional terms, normally if you take say heat transfer applications you do not have this particular term basically, but now the enthalpy transport due to the species diffusion is also one of the important thing.

The enthalpy when you calculate, it is just c_p×T in the heat transfer application, but you can see the enthalpy of formation comes here due to the reactive nature of the system.

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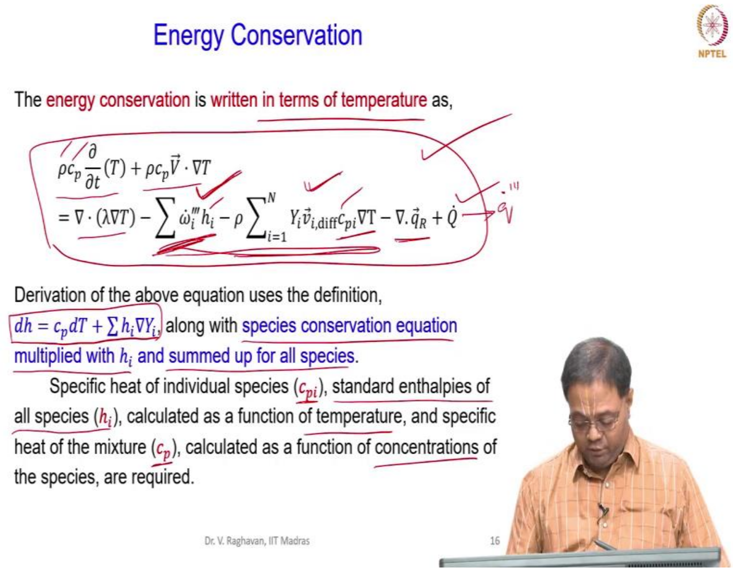

Energy Conservation

The energy conservation is written in terms of temperature as,

$$\rho c_p \frac{\partial}{\partial t}(T) + \rho c_p \vec{V} \cdot \nabla T = \nabla \cdot (\lambda \nabla T) - \sum \dot{\omega}_i''' h_i - \rho \sum_{i=1}^{N} Y_i \vec{v}_{i,\mathrm{diff}} c_{pi} \nabla T - \nabla . \vec{q}_R + \dot{Q} \rightarrow \dot{q}'''$$

Derivation of the above equation uses the definition, $dh = c_p dT + \sum h_i \nabla Y_i$, along with species conservation equation multiplied with h_i and summed up for all species.

Specific heat of individual species (c_{pi}), standard enthalpies of all species (h_i), calculated as a function of temperature, and specific heat of the mixture (c_p), calculated as a function of concentrations of the species, are required.

Now, in terms of temperature. When you want to write in terms of temperature, we have to use definition like this, $dh = c_p dT + h_i \nabla Y_i$. The change in the specific enthalpy of the mixture will be the mixture specific heat into dT.

So, this itself, c_p of the mixture itself will be a function of temperature. So, this you have to integrate basically plus integral $\int h_i \nabla Y_i$. So, this is the second term which I have to add. Then, we have to use species conservation equation multiplied by h_i and summed up all the species if you take species conservation equation, for each species multiply that by h_i overall.

Then, add up for all the species, then you will get this and this combined together you can write this equation. Here, you see that the ρ (mixture density) c_p (of the mixture) × $\partial u / \partial T$ + $\rho c_p \vec{V} . \nabla T$ this is the convective term here.

So, now enthalpy is expanded and the energy equation is written in terms of temperature.

$$\begin{aligned} \rho c_p \frac{\partial}{\partial t}(T) + \rho c_p \vec{V} \cdot \nabla T \\ &= \nabla \cdot (\lambda \nabla T) - \sum \dot{\omega}_i''' h_i \\ &- \rho \sum_{i=1}^{N} Y_i \vec{v}_{i,\mathrm{diff}} c_{pi} \nabla \mathrm{T} - \nabla . \vec{q}_R + \dot{Q} \end{aligned}$$

So, now, that will be equal to the gradient of the conduction flux plus this.

So, you can see I am using this species conservation equation multiplied by h_i and summed up for all the species, so that will give this term. The source term of each species is the rate at which the species is consumed or produced. So, $\dot{\omega}_i'''$. So, that is the volumetric source term that into h_i. So, I am multiplying the species conversion equation by the h_i and summing up. So, that summed up term is the term here that comes out as a source term.

Similarly, the flux term remains like this. But here instead of writing enthalpy I am writing $c_{pi} \nabla T$, c_{pi} of each species and gradient of temperature. Previously we wrote h_i, instead of h_i I am now writing as c_{pi} into gradient of temperature plus the flux due to the radiation source term.

This is the volumetric source term I have written here. So, these are the things, this actually in the previous slide it was written as this is same as this. So, now, you can see that you get the volumetric source term basically which is non-linear in nature. So, this is one of the important additions.

So, these two are the terms which is important for the reactive flows, the energy transport due to diffusion of species. Similarly, the energy generated due to the volumetric reactions of each species. So, these two terms are important for the reactive flows.

Other terms you can see in general heat transfer applications. So, the entire derivation is not given here, but to derive from this enthalpy based energy conservation, we have to use this definition dh = c_p dT + $h_i \nabla Y_i$.

Then, species conservation equation for each species multiplied by h_i, its own enthalpy, specific enthalpy and summed up for all the species that will give rise to this equation which is written in terms of temperature. So, that is a primitive variable we want in terms of temperature. So, when you write the equation in this term then you can directly solve for the temperature.

Now, please see that for energy equation, you need individual species now you can see that c_{pi} is involved. So, specific heat at constant pressure for individual species is required. Then, h_i, standard or absolute enthalpies of all the species is required. These have to be calculated as a function of temperature basically. Then, specific heat of the mixture at constant pressure c_p. This has to be calculated as a function of concentrations as well as temperature both.

Now, ρ is calculated using the equation of state. So, this is the consolidated energy equation. Please understand in this we have neglected the work interactions due to pressure force, viscous dissipation, and the body forces.