Turbulent Combustion: Theory and Modelling
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Lecture-43
Turbulence - Chemistry Interaction (contd...)

Welcome back. So, let us continue the discussion on turbulent combustion. So, we are looking at the different governing equations and the one which we were doing right now, the discussion is the conservation equation of the total energy.

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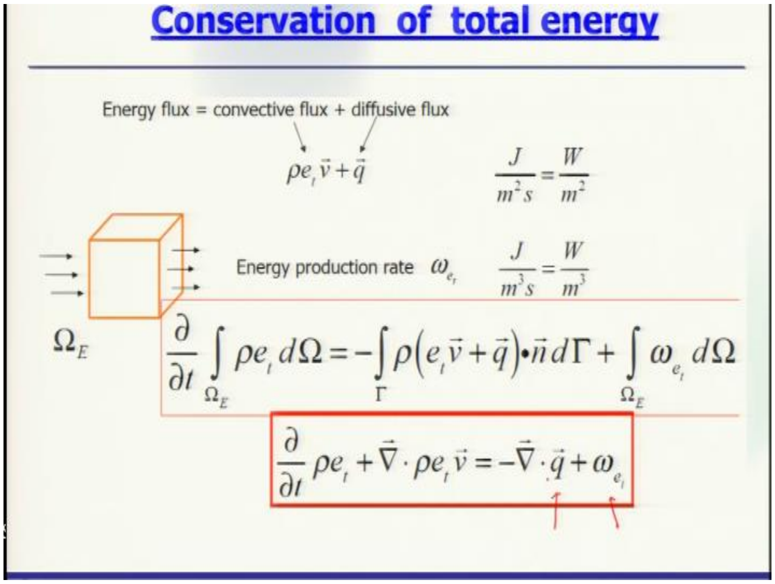

Conservation of total energy

Energy flux = convective flux + diffusive flux

$\rho e_t \vec{v} + \vec{q}$ $\qquad \frac{J}{m^2 s} = \frac{W}{m^2}$

Energy production rate ω_{e_t} $\qquad \frac{J}{m^3 s} = \frac{W}{m^3}$

Ω_E

$$\frac{\partial}{\partial t}\int_{\Omega_E} \rho e_t \, d\Omega = -\int_{\Gamma} \rho\left(e_t \vec{v} + \vec{q}\right)\bullet \vec{n} \, d\Gamma + \int_{\Omega_E} \omega_{e_t} \, d\Omega$$

$$\boxed{\frac{\partial}{\partial t}\rho e_t + \vec{\nabla}\cdot \rho e_t \vec{v} = -\vec{\nabla}\cdot \vec{q} + \omega_{e_t}}$$

So, this is how the total energy equation would look like. When you look at the control volume and the different terminology we have discussed. So, here there are 2 components, one is this component and the other is this component.

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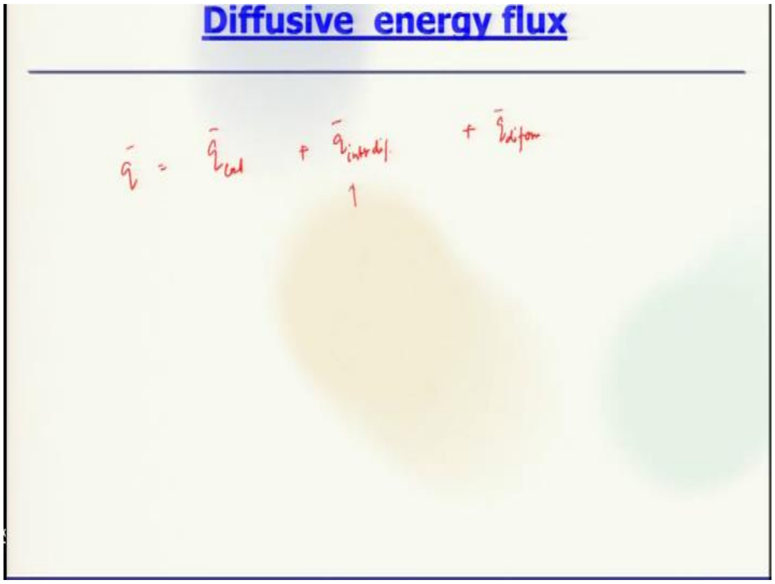

Diffusive energy flux

$$\bar{q} = \bar{q}_{cond} + \bar{q}_{interdif} + \bar{q}_{dufor}$$

$\uparrow$

Now, we have already looked at this q, there are 3 components one could be due to conduction, then interdiffusion, and finally the Dufour effect, but this is due to conduction in flux and this is due to species diffusion and this is due to gradient in species concentration, that will look at the anonymous number and all these.

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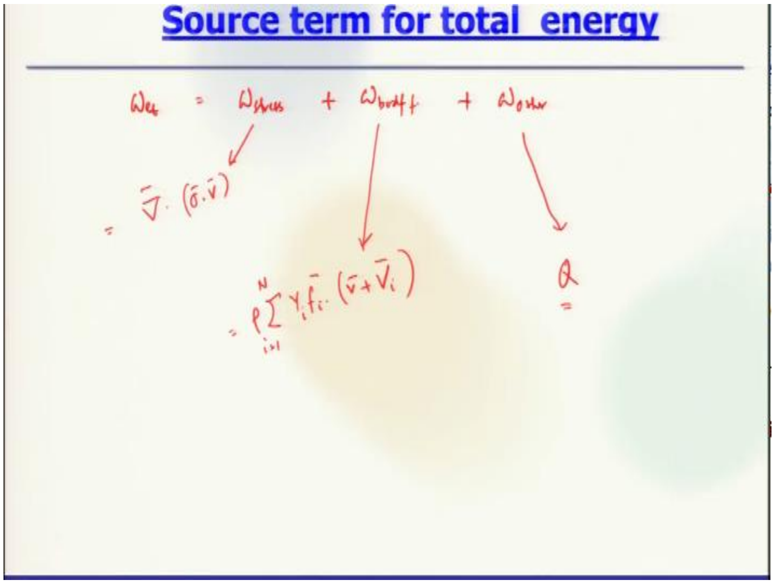

Source term for total energy

$$\omega_{et} = \omega_{stress} + \omega_{bodyf} + \omega_{other}$$

$$= \bar{\nabla}\cdot(\bar{\sigma}\cdot\bar{v})$$

$$= \rho\sum_{i=1}^{N} Y_i \bar{f}_i \cdot (\bar{v}+\bar{V}_i)$$

$$Q$$

$$=$$

So, now we will look at the source term of the total energy that is W_{et} there would be stress component plus there would be body force and there would be components if there are any other sources. So, the stress component one can represent that $\bar{\nabla}(\bar{\sigma}.\ \bar{v})$, which is the one by stresses. body force component one can represent like $\rho \sum_{i+1}^{N} Y_i \bar{f_i}\ (\bar{v} + \bar{V_i}\ )$. This is the work done due to body forces and the other sources one can keep it Q this could be source or symptom, let us say.

If you have radiation effect and some other effects, which would provide some source term, so, that can be taken into consideration under the term. So, one has to note where there is no source due to heat by the reaction. So, this is one can note that and that is it because, that is it transformation between 2 forms of energy, both continue in internal energy which is in chemical and thermal.

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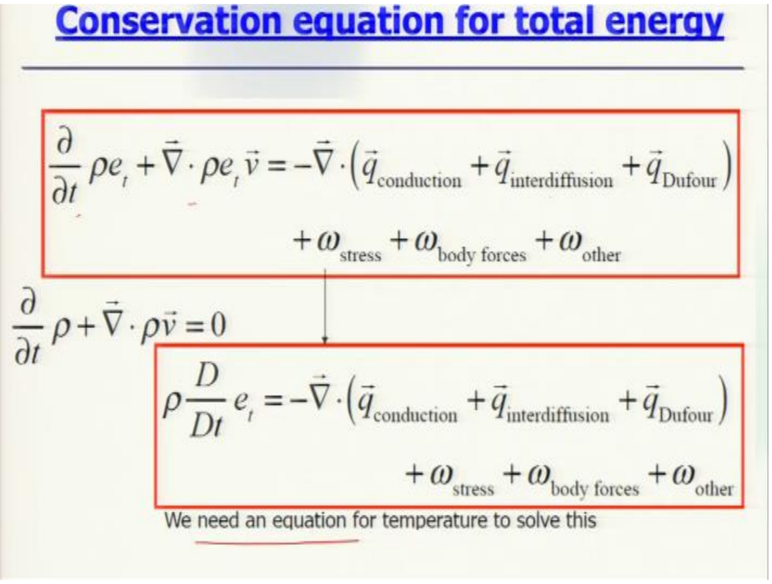

Conservation equation for total energy

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}\rho e_t + \vec{\nabla}\cdot\rho e_t\vec{v} &= -\vec{\nabla}\cdot\left(\vec{q}_{\text{conduction}} + \vec{q}_{\text{interdiffusion}} + \vec{q}_{\text{Dufour}}\right)\\ &\quad + \omega_{\text{stress}} + \omega_{\text{body forces}} + \omega_{\text{other}}\end{aligned}}$$

$$\frac{\partial}{\partial t}\rho + \vec{\nabla}\cdot\rho\vec{v} = 0$$

$$\boxed{\begin{aligned}\rho\frac{D}{Dt}e_t &= -\vec{\nabla}\cdot\left(\vec{q}_{\text{conduction}} + \vec{q}_{\text{interdiffusion}} + \vec{q}_{\text{Dufour}}\right)\\ &\quad + \omega_{\text{stress}} + \omega_{\text{body forces}} + \omega_{\text{other}}\end{aligned}}$$

We need an equation for temperature to solve this

So, if you include everything together the equation would look like this is my answer term convection term, this is the flux due to conduction, the diffusion, Dufour, source term like this and which can be written like this also. So, now this is we need another equation for the temperature to solve this.

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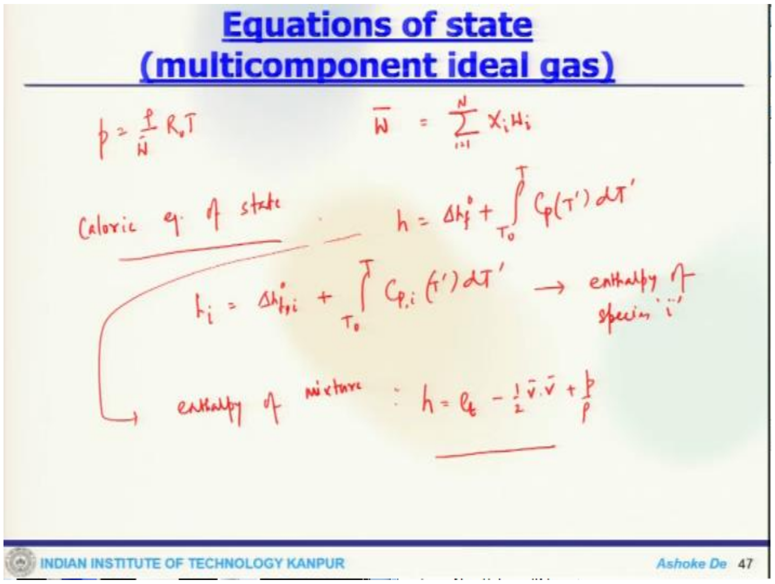

Equations of state
(multicomponent ideal gas)

$p = \frac{\rho}{\bar{W}} R_o T$ $\quad \bar{W} = \sum_{i=1}^{N} X_i W_i$

Caloric eq. of state $\quad h = \Delta h_f^0 + \int_{T_0}^{T} C_p(T')\,dT'$

$h_i = \Delta h_{f,i}^0 + \int_{T_0}^{T} C_{p,i}(T')\,dT' \rightarrow$ enthalpy of species 'i'

enthalpy of mixture : $h = e_t - \frac{1}{2}\bar{v}.\bar{v} + \frac{p}{\rho}$

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So, we invoke the equation of state. So, one is the thermodynamical equation of state where

$$p = \frac{\rho}{\bar{W}} R_o T$$

so that will relate pressure, molar density, and temperature, and $\bar{W}$ is a mixture molecular weight which would be

$$\bar{W} = \sum_{i+1}^{N} X_i W_i$$

$X_i W_i$ apart from this we need the caloric equation of state which will give us

$$h = \Delta h_f^0 + \int_{T_o}^{T} C_p(T')dT'$$

here

$$h_i = \Delta h_{f,i}^0 + \int_{T_o}^{T} C_{p,i}(T')dT'$$

So, this is enthalpy of species i and this is essentially the enthalpy of mixture h one can right it like this

$$h = e_t - \frac{1}{2}\bar{v}.\bar{v} + \frac{p}{\rho}$$

So, once we write this from here, we can estimate the temperature from this.

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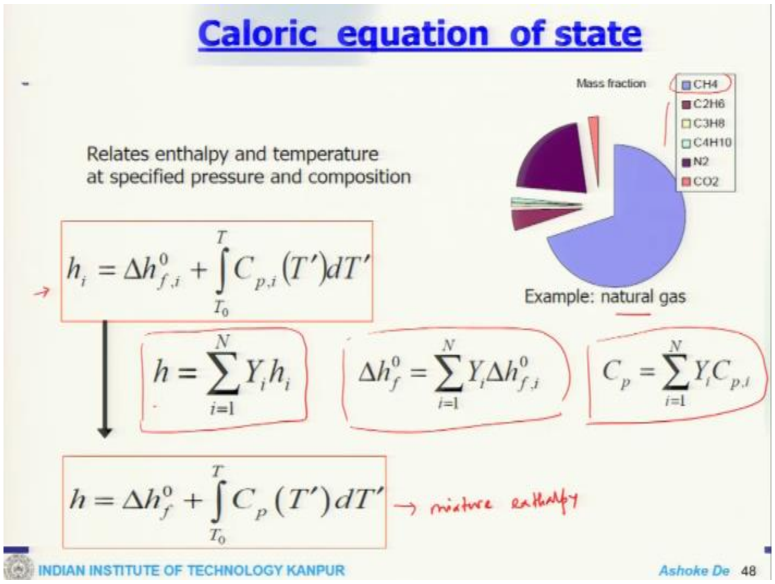

Caloric equation of state

Relates enthalpy and temperature
at specified pressure and composition

Example: natural gas

$$\rightarrow \boxed{h_i = \Delta h^0_{f,i} + \int_{T_0}^{T} C_{p,i}(T')dT'}$$

$$h = \sum_{i=1}^{N} Y_i h_i \qquad \Delta h^0_f = \sum_{i=1}^{N} Y_i \Delta h^0_{f,i} \qquad C_p = \sum_{i=1}^{N} Y_i C_{p,i}$$

$$\boxed{h = \Delta h^0_f + \int_{T_0}^{T} C_p(T')dT'} \rightarrow \text{mixture enthalpy}$$

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Now, more how this caloric equation of state. So, these are the multi-component mixture, which is an example of natural gas whereby large CH_4 is there than other components are there. So, this relates the enthalpy and temperature for a given pressure and composition. So, this is your individual species enthalpy.

And from there, this is my mixture enthalpy now, one can also get that one by getting

$$h = \sum_{i=1}^{N} Y_i h_i$$

hSo that is also can be used where Δh_f^0 is the summation of all the species and C_p is like that. So, these setup equations are also evaluated and for multi-component mixture, one can use that.

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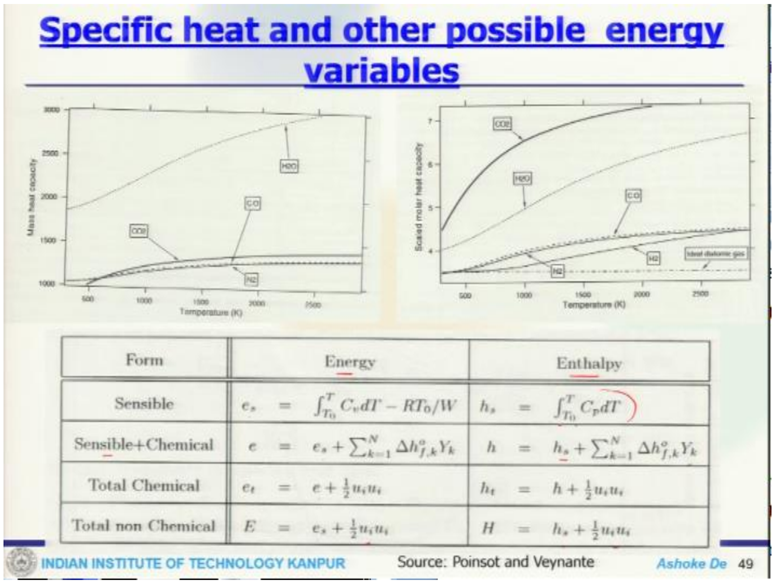

Specific heat and other possible energy variables

Form	Energy	Enthalpy
Sensible	$e_s = \int_{T_0}^{T} C_v dT - RT_0/W$	$h_s = \int_{T_0}^{T} C_p dT$
Sensible+Chemical	$e = e_s + \sum_{k=1}^{N} \Delta h_{f,k}^o Y_k$	$h = h_s + \sum_{k=1}^{N} \Delta h_{f,k}^o Y_k$
Total Chemical	$e_t = e + \frac{1}{2} u_i u_i$	$h_t = h + \frac{1}{2} u_i u_i$
Total non Chemical	$E = e_s + \frac{1}{2} u_i u_i$	$H = h_s + \frac{1}{2} u_i u_i$

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Now, if you look at the specific heat and other possible energy variables and have an idea of how that varies. So, you look at here the mass heat capacity. This is the scaled molar heat capacity this is varying with temperature. So, this picture is adapted from the book from the Poinsot and Veynante, this is for different mixture, you can see how that varies provided here temperature same thing. So, if you put all these different forms of energy then we can see the relationship between energy and the enthalpy.

So, the sensible energy one can write e_s which stands for sensible energy, which is

$$e_s = \int_{T_o}^{T} C_v dT - RT_o/W$$

So, that this component $\int_{T_o}^{T} C_v dT$ would the integration of provide the sensible enthalpy. Now, once we add sensible plus chemical, so here the energy component that e_s coming from sensible and then this is the component due to the chemical energy that individual change in enthalpy for individual species and the sum of there all the species.

So, and in terms of enthalpy there would be a component coming from the sensible one and this is the component into chemical one. So, the total chemical would be

$$e_t = e + \frac{1}{2} u_i u_i$$

and h_t would be

$$h_t = h + \frac{1}{2} u_i u_i$$

and non-chemical sensible plus kinetic energy this is sensible plus kinetic energy. So, this is a relation that one can see.

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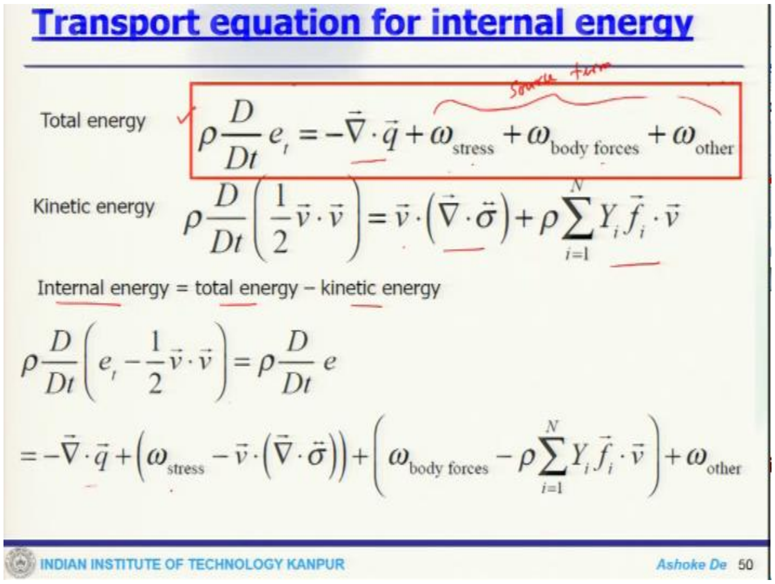

Transport equation for internal energy

Source term

Total energy $$\boxed{\rho\frac{D}{Dt}e_t = -\vec{\nabla}\cdot\vec{q} + \omega_{\text{stress}} + \omega_{\text{body forces}} + \omega_{\text{other}}}$$

Kinetic energy $$\rho\frac{D}{Dt}\left(\frac{1}{2}\vec{v}\cdot\vec{v}\right) = \vec{v}\cdot\left(\vec{\nabla}\cdot\vec{\sigma}\right) + \rho\sum_{i=1}^{N}Y_i\vec{f}_i\cdot\vec{v}$$

Internal energy = total energy − kinetic energy

$$\rho\frac{D}{Dt}\left(e_t - \frac{1}{2}\vec{v}\cdot\vec{v}\right) = \rho\frac{D}{Dt}e$$

$$= -\vec{\nabla}\cdot\vec{q} + \left(\omega_{\text{stress}} - \vec{v}\cdot\left(\vec{\nabla}\cdot\vec{\sigma}\right)\right) + \left(\omega_{\text{body forces}} - \rho\sum_{i=1}^{N}Y_i\vec{f}_i\cdot\vec{v}\right) + \omega_{\text{other}}$$

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Now, we can write the transport equation in terms of internal energy. So, this is the conservation equation where left-hand side is the total derivative of that and we have the flux gradient of the flux and the body forces term or the source term. So, this is essentially our source term. Now, this is stress component, body force component, and other components.

Now, kinetic energy one can write that total kinetic energy is a derivative of the kinetic energy source term and this. So, one can find out the internal energy equals to total energy minus kinetic energy. So, this is what we get

$$\rho\frac{De_t}{Dt} = -\vec{\nabla}.\vec{q} + \omega_{stress} + \omega_{body\ forces} + \omega_{other}$$

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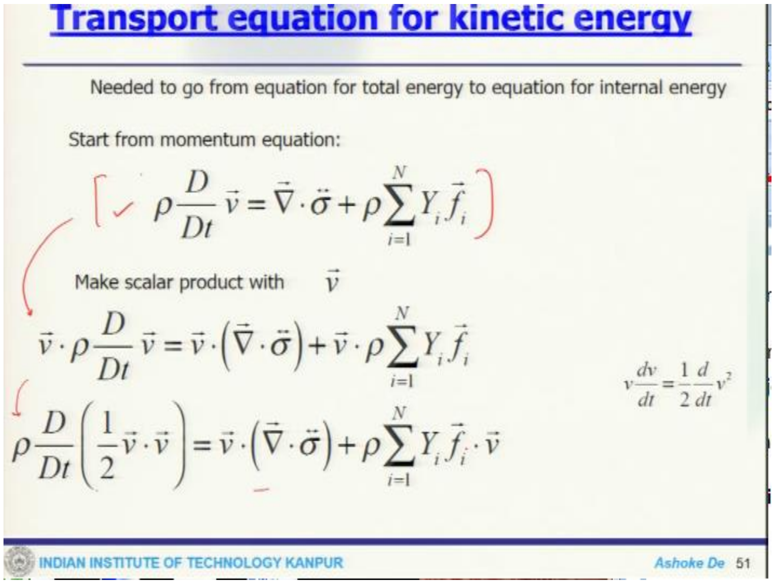

Transport equation for kinetic energy

Needed to go from equation for total energy to equation for internal energy

Start from momentum equation:

$$\rho\frac{D}{Dt}\vec{v} = \vec{\nabla}\cdot\vec{\sigma} + \rho\sum_{i=1}^{N} Y_i\vec{f}_i$$

Make scalar product with $\vec{v}$

$$\vec{v}\cdot\rho\frac{D}{Dt}\vec{v} = \vec{v}\cdot\left(\vec{\nabla}\cdot\vec{\sigma}\right) + \vec{v}\cdot\rho\sum_{i=1}^{N} Y_i\vec{f}_i$$

$$\rho\frac{D}{Dt}\left(\frac{1}{2}\vec{v}\cdot\vec{v}\right) = \vec{v}\cdot\left(\vec{\nabla}\cdot\vec{\sigma}\right) + \rho\sum_{i=1}^{N} Y_i\vec{f}_i\cdot\vec{v}$$

$$v\frac{dv}{dt} = \frac{1}{2}\frac{d}{dt}v^2$$

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So, one can go for the equation of total energy to the equation of internal energy. So, one can start from the momentum equation, which will give you the Navier-Stokes equations . So, multiply this one with the v of the scalar product of that. So, this equation will be taken scalar product and that will give me this.

$$\vec{v}\rho\frac{D\vec{v}}{Dt} = \vec{v}.\left(\vec{\nabla}\,\bar{\sigma}\,\right) + \vec{v}.\rho\sum_{i=1}^{N} Y_i\overrightarrow{f_i}$$

Now, here we can rewrite the left hand side term likes this right hand side like this and the other term in this fashion.

$$\rho\frac{D\left(\frac{1}{2}\vec{v}.\,\vec{v}\right)}{Dt} = \vec{v}.\left(\vec{\nabla}\,\bar{\sigma}\,\right) + \rho\sum_{i=1}^{N} Y_i\overrightarrow{f_i}\,\vec{v}$$

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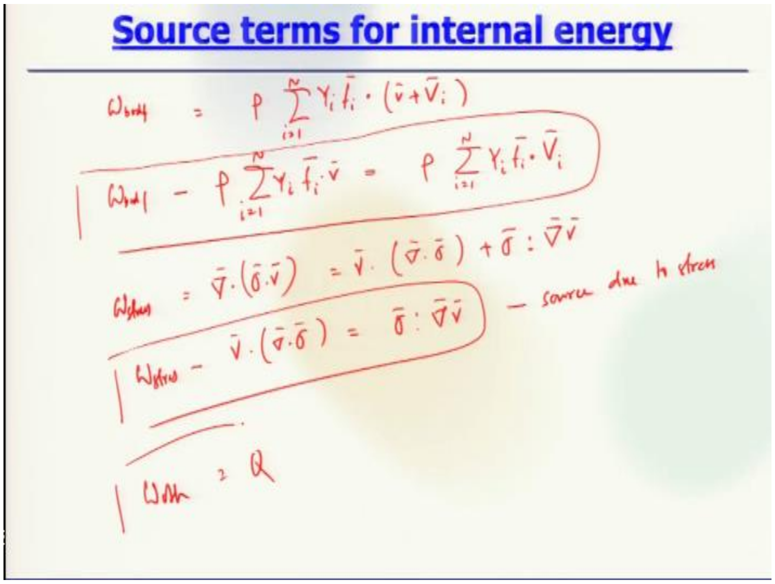

Source terms for internal energy

$$W_{body} = \rho \sum_{i=1}^{N} Y_i \bar{f}_i \cdot (\bar{v} + \bar{V}_i)$$

$$W_{body} - \rho \sum_{i=1}^{N} Y_i \bar{f}_i \cdot \bar{v} = \rho \sum_{i=1}^{N} Y_i \bar{f}_i \cdot \bar{V}_i$$

$$W_{stress} = \bar{\nabla} \cdot (\bar{\sigma} \cdot \bar{v}) = \bar{v} \cdot (\bar{\nabla} \cdot \bar{\sigma}) + \bar{\sigma} : \bar{\nabla} \bar{v}$$

$$W_{stress} - \bar{v} \cdot (\bar{\nabla} \cdot \bar{\sigma}) = \bar{\sigma} : \bar{\nabla} \bar{v}$$ — source due to stress

$$W_{other} = Q$$

So, look at the source term for that we have body force which is

$$W_{body} - \rho \sum_{i=1}^{N} Y_i \overrightarrow{f_i}\, \vec{v} = \sum_{i=1}^{N} Y_i \overrightarrow{f_i}\, \vec{V_i}$$

So one can write that. So this source due to product and the first deficient velocity.

Now,

$$W_{stress} = \overline{\nabla}\,(\bar{\sigma}.\bar{v}) = \bar{v}(\overline{\nabla}\bar{\sigma}) + \bar{\sigma}\,\overline{\nabla}\,\bar{v}$$

where one can write

$$W_{stress} - \bar{v}(\overline{\nabla}\bar{\sigma}) = \bar{\sigma}\,\overline{\nabla}\,\bar{v} - \mathit{source\ due\ to\ stress}$$

So, that is why tensor product. So, this is a source due to stress and other would be Q this is source due to other terms.

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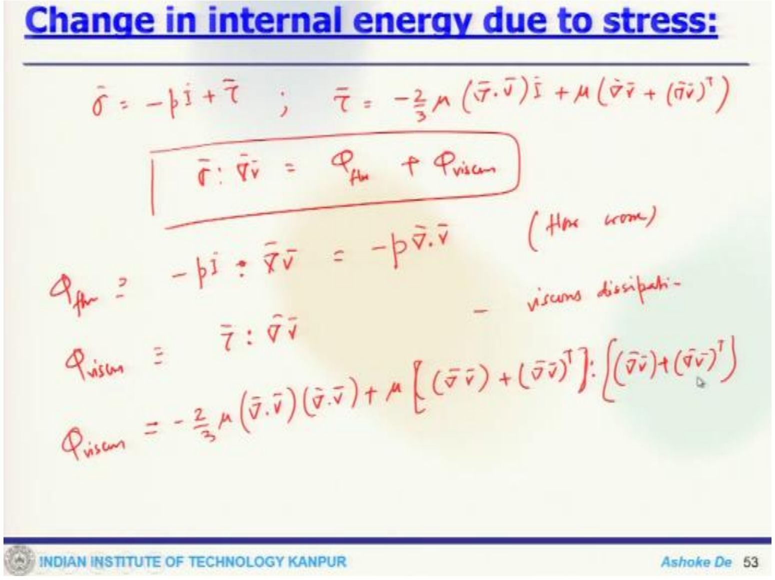

Change in internal energy due to stress:

$$\bar{\sigma} = -pI + \bar{\tau} \quad ; \quad \bar{\tau} = -\frac{2}{3}\mu(\bar{\nabla}.\bar{v})I + \mu(\bar{\nabla}\bar{v} + (\bar{\nabla}\bar{v})^T)$$

$$\boxed{\bar{\sigma} : \bar{\nabla}\bar{v} = \phi_{flow} + \phi_{viscous}}$$

$$\phi_{flow} = -pI : \bar{\nabla}\bar{v} = -p\bar{\nabla}.\bar{v} \quad (\text{flow work})$$

$$\phi_{viscous} = \bar{\tau} : \bar{\nabla}\bar{v} \quad - \text{viscous dissipation}$$

$$\phi_{viscous} = -\frac{2}{3}\mu(\bar{\nabla}.\bar{v})(\bar{\nabla}.\bar{v}) + \mu\left[(\bar{\nabla}\bar{v}) + (\bar{\nabla}\bar{v})^T\right] : \left[(\bar{\nabla}\bar{v}) + (\bar{\nabla}\bar{v})^T\right)$$

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Now, one can look at the change in the energy internal energy due to stress. So, the sigma is written as

$$\bar{\sigma} = -pI + \bar{\tau}$$

where

$$\bar{\tau} = -\frac{2}{3}\mu(\overline{\nabla}.\bar{v})I + \mu(\overline{\nabla}.\bar{v} + (\overline{\nabla}.\bar{v})^{\tau})$$

So, the tensor product of that would be

$$\bar{\sigma}\overline{\nabla}.\bar{v} = \phi_{flow} + \phi_{viscous}$$

so, this is an important correlation and sigma flow for this is

$$\phi_{flow} = -pI\overline{\nabla}.\bar{v} = -p\overline{\nabla}.\bar{v}$$

$$\phi_{viscous} = \bar{\tau}\overline{\nabla}.\bar{v}$$

$$\phi_{viscous} == -\frac{2}{3}\mu(\overline{\nabla}.\bar{v})(\overline{\nabla}.\bar{v}) + \mu(\overline{\nabla}.\bar{v} + (\overline{\nabla}.\bar{v})^{\tau})(\overline{\nabla}.\bar{v} + (\overline{\nabla}.\bar{v})^{\tau})$$

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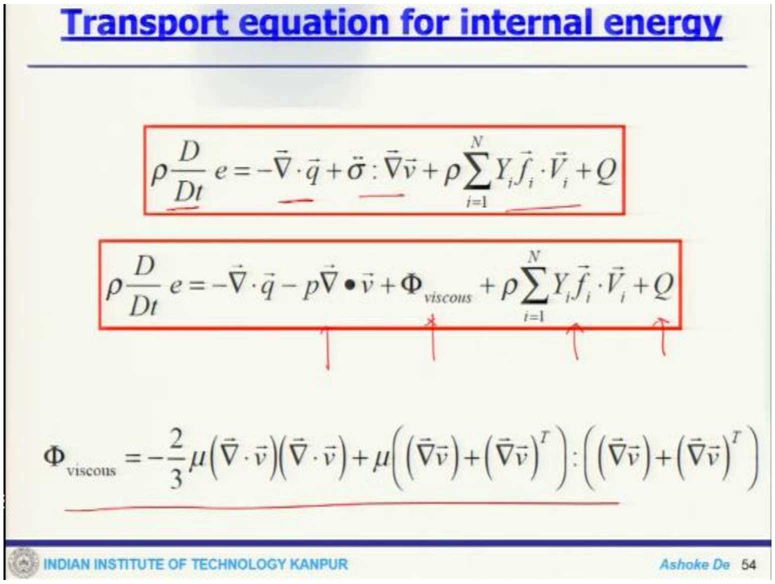

Transport equation for internal energy

$$\boxed{\rho \frac{D}{Dt} e = -\vec{\nabla}\cdot\vec{q} + \vec{\sigma}:\vec{\nabla}\vec{v} + \rho\sum_{i=1}^{N} Y_i \vec{f}_i\cdot\vec{V}_i + Q}$$

$$\boxed{\rho \frac{D}{Dt} e = -\vec{\nabla}\cdot\vec{q} - p\vec{\nabla}\bullet\vec{v} + \Phi_{viscous} + \rho\sum_{i=1}^{N} Y_i \vec{f}_i\cdot\vec{V}_i + Q}$$

$$\Phi_{\text{viscous}} = -\frac{2}{3}\mu\left(\vec{\nabla}\cdot\vec{v}\right)\left(\vec{\nabla}\cdot\vec{v}\right) + \mu\left(\left(\vec{\nabla}\vec{v}\right)+\left(\vec{\nabla}\vec{v}\right)^{T}\right):\left(\left(\vec{\nabla}\vec{v}\right)+\left(\vec{\nabla}\vec{v}\right)^{T}\right)$$

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Transport equation if I look at it finally, for the internal energy, this is the term left-hand side total derivative flux stress and another term is just similar that, so, this will get to viscous this term, other source term process stress in this at the viscous of this it will get like that.

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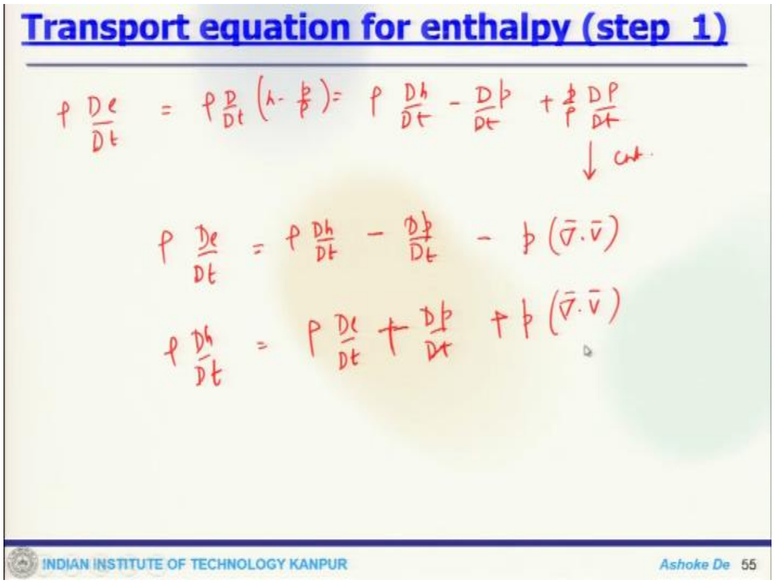

Transport equation for enthalpy (step 1)

$$\rho \frac{De}{Dt} = \rho\frac{D}{Dt}\left(h - \frac{p}{\rho}\right) = \rho\frac{Dh}{Dt} - \frac{Dp}{Dt} + \frac{p}{\rho}\frac{D\rho}{Dt}$$

$\downarrow$ cont.

$$\rho\frac{De}{Dt} = \rho\frac{Dh}{Dt} - \frac{Dp}{Dt} - p\left(\vec{\nabla}\cdot\vec{v}\right)$$

$$\rho\frac{Dh}{Dt} = \rho\frac{De}{Dt} + \frac{Dp}{Dt} + p\left(\vec{\nabla}\cdot\vec{v}\right)$$

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Now, similarly, one can derive the transport equation for enthalpy. So how do we do that, we actually write this equation, which is

$$\rho\frac{De}{Dt} = \rho\frac{D}{Dt}\left(h - \frac{p}{\rho}\right) = \rho\frac{Dh}{Dt} - \frac{Dp}{Dt} + \frac{p}{\rho}\frac{Dp}{Dt}$$

So, this is essentially our continuity equation. So one can write

$$\rho\frac{De}{Dt} = \rho\frac{Dh}{Dt} - \frac{Dp}{Dt} - p(\overline{\nabla}.\vec{v})$$

$$\rho\frac{Dh}{Dt} = \rho\frac{De}{Dt} + \frac{Dp}{Dt} + p(\overline{\nabla}.\vec{v})$$

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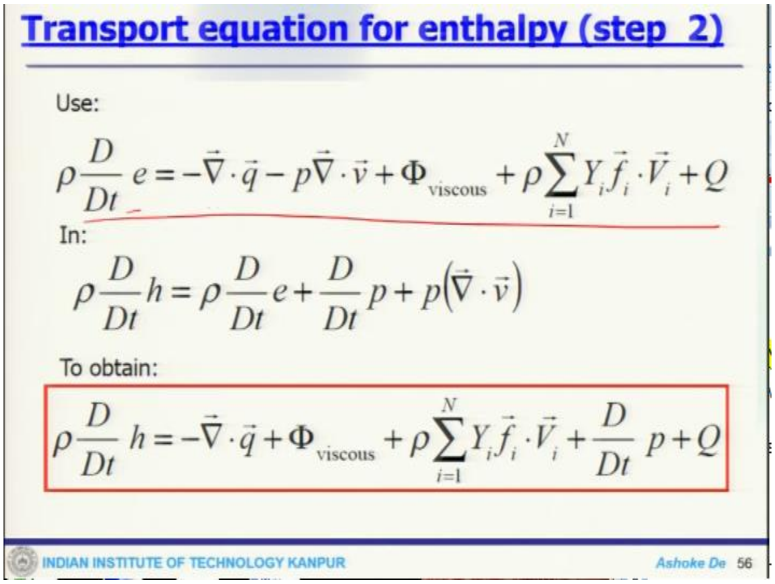

Transport equation for enthalpy (step 2)

Use:

$$\rho\frac{D}{Dt}e = -\vec{\nabla}\cdot\vec{q} - p\vec{\nabla}\cdot\vec{v} + \Phi_{\text{viscous}} + \rho\sum_{i=1}^{N} Y_i\vec{f}_i\cdot\vec{V}_i + Q$$

In:

$$\rho\frac{D}{Dt}h = \rho\frac{D}{Dt}e + \frac{D}{Dt}p + p\left(\vec{\nabla}\cdot\vec{v}\right)$$

To obtain:

$$\boxed{\rho\frac{D}{Dt}h = -\vec{\nabla}\cdot\vec{q} + \Phi_{\text{viscous}} + \rho\sum_{i=1}^{N} Y_i\vec{f}_i\cdot\vec{V}_i + \frac{D}{Dt}p + Q}$$

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So, now, use:

$$\rho\frac{De}{Dt} = -\vec{\nabla}.\vec{q} - p\vec{\nabla}.\vec{v} + \Phi_{viscous} + \rho\sum_{i=1}^{N} Y_i\vec{f_i}\vec{V_i} + Q$$

In:

$$\rho\frac{Dh}{Dt} = \rho\frac{De}{Dt} + \frac{Dp}{Dt} + p(\vec{\nabla}.\vec{v})$$

To obtain:

$$\rho\frac{Dh}{Dt} = -\vec{\nabla}.\vec{q} + \Phi_{viscous} + \rho\sum_{i=1}^{N} Y_i\vec{f_i}\vec{V_i} + \frac{Dp}{Dt} + Q$$

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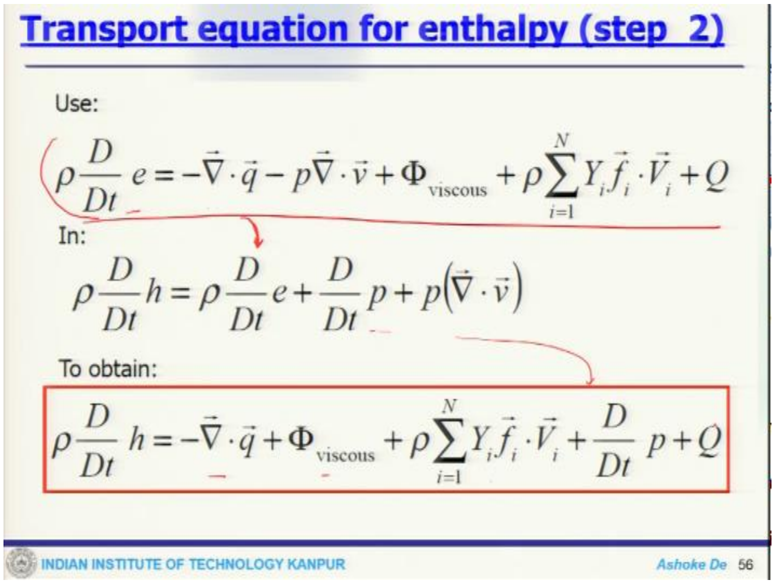

Transport equation for enthalpy (step 2)

Use:

$$\rho \frac{D}{Dt} e = -\vec{\nabla}\cdot\vec{q} - p\vec{\nabla}\cdot\vec{v} + \Phi_{\text{viscous}} + \rho\sum_{i=1}^{N} Y_i \vec{f}_i \cdot \vec{V}_i + Q$$

In:

$$\rho \frac{D}{Dt} h = \rho \frac{D}{Dt} e + \frac{D}{Dt} p + p\left(\vec{\nabla}\cdot\vec{v}\right)$$

To obtain:

$$\boxed{\rho \frac{D}{Dt} h = -\vec{\nabla}\cdot\vec{q} + \Phi_{\text{viscous}} + \rho\sum_{i=1}^{N} Y_i \vec{f}_i \cdot \vec{V}_i + \frac{D}{Dt} p + Q}$$

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So, if you use this one this expression back in here, then we get

$$\rho\frac{Dh}{Dt} = -\vec{\nabla}.\vec{q} + \Phi_{viscous} + \rho\sum_{i=1}^{N} Y_i \overrightarrow{f_i}\overrightarrow{V_i} + \frac{Dp}{Dt} + Q$$

then this term will remain as it is and we have the source term coming in.

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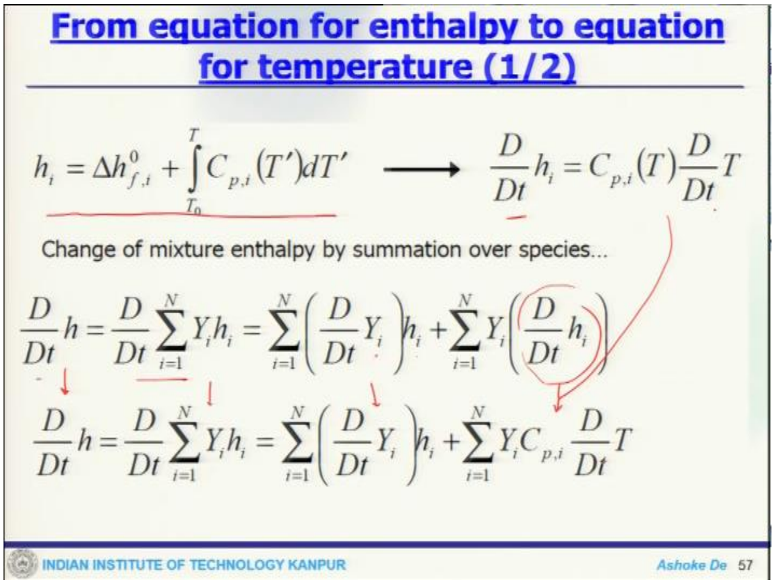

From equation for enthalpy to equation for temperature (1/2)

$$h_i = \Delta h^0_{f,i} + \int_{T_0}^{T} C_{p,i}(T')dT' \longrightarrow \frac{D}{Dt}h_i = C_{p,i}(T)\frac{D}{Dt}T$$

Change of mixture enthalpy by summation over species...

$$\frac{D}{Dt}h = \frac{D}{Dt}\sum_{i=1}^{N} Y_i h_i = \sum_{i=1}^{N}\left(\frac{D}{Dt}Y_i\right)h_i + \sum_{i=1}^{N} Y_i\left(\frac{D}{Dt}h_i\right)$$

$$\frac{D}{Dt}h = \frac{D}{Dt}\sum_{i=1}^{N} Y_i h_i = \sum_{i=1}^{N}\left(\frac{D}{Dt}Y_i\right)h_i + \sum_{i=1}^{N} Y_i C_{p,i}\frac{D}{Dt}T$$

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So, now, we can see that how we evaluate the temperature from the enthalpy equation, we have individual species enthalpy. Then from there if we take the derivative of that, this will be

$$\frac{Dh_i}{Dt} = C_{p,i}(T)\frac{DT}{Dt}$$

a change of mixture enthalpy by sum our all the species so, Dh/DT if you take the sum. So, this will be sum our

$$\frac{Dh}{Dt} = \frac{D}{Dt}\sum_{i=1}^{N} Y_i h_i = \sum_{i=1}^{N}\left(\frac{D}{Dt}Y_i\right)h_i + Y\sum_{i=1}^{N}\left(\frac{D}{Dt}h_{i_{i}}\right)$$

if we take the derivative the first term, so, this will be the total derivative of mass fraction multiplied by individual enthalpy mass fraction taking individual derivative of the enthalpy.

So, Dh/Dt will come like this time remain as it is, and here we change this particular term we will replace with this, so that we get

$$\frac{Dh}{Dt} = \frac{D}{Dt}\sum_{i=1}^{N} Y_i h_i = \sum_{i=1}^{N}\left(\frac{D}{Dt}Y_i\right)h_i + Y\sum_{i=1}^{N} Y_i C_{p,i}(T)\frac{DT}{Dt}$$

So, this is a nothing but the algebra.

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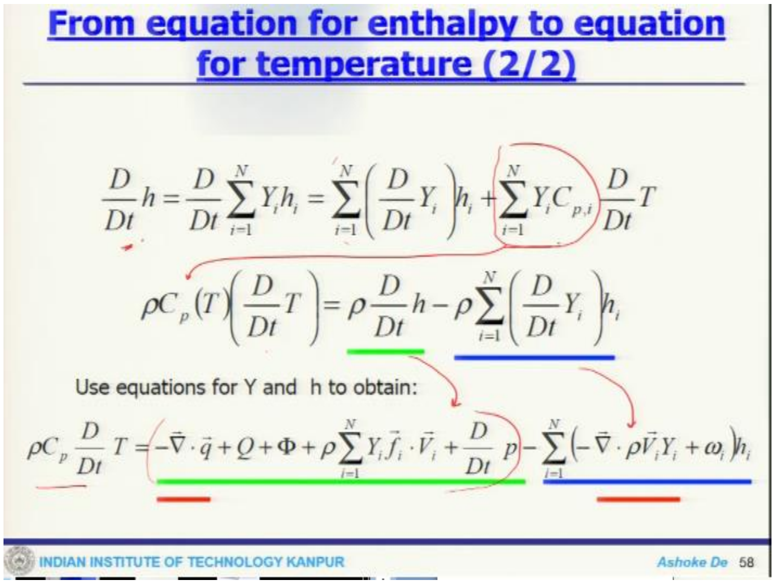

From equation for enthalpy to equation for temperature (2/2)

$$\frac{D}{Dt}h = \frac{D}{Dt}\sum_{i=1}^{N} Y_i h_i = \sum_{i=1}^{N}\left(\frac{D}{Dt}Y_i\right)h_i + \sum_{i=1}^{N} Y_i C_{p,i}\frac{D}{Dt}T$$

$$\rho C_p(T)\left(\frac{D}{Dt}T\right) = \rho\frac{D}{Dt}h - \rho\sum_{i=1}^{N}\left(\frac{D}{Dt}Y_i\right)h_i$$

Use equations for Y and h to obtain:

$$\rho C_p\frac{D}{Dt}T = -\vec{\nabla}\cdot\vec{q} + Q + \Phi + \rho\sum_{i=1}^{N} Y_i\vec{f}_i\cdot\vec{V}_i + \frac{D}{Dt}p - \sum_{i=1}^{N}\left(-\vec{\nabla}\cdot\rho\vec{V}_i Y_i + \omega_i\right)h_i$$

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Now, we write Dh/Dt, we keep this term as it is and this term. So, here if we look at

$$\rho C_p(T)\left(\frac{DT}{Dt}\right) = \rho\frac{Dh}{Dt} - \rho\sum_{i=1}^{N}\left(\frac{D}{Dt}Y_i\right)h_i$$

this essentially the sum of all these things, this will get me Cp that is the mixture Cp all that which are obtain.

So, now, you can use the equation of Y and h to obtain a temperature equation. So, that will give me

$$\rho C_p(T)\left(\frac{DT}{Dt}\right) == -\vec{\nabla}.\vec{q} + Q + \Phi + \rho\sum_{i=1}^{N} Y_i\overrightarrow{f_i}\overrightarrow{V_i} + \frac{Dp}{Dt} - \sum_{i=1}^{N}(\vec{\nabla}.\rho\overrightarrow{V_i}Y_i + \omega_i)h_i$$

So, this one is coming from my these things this guy will contribute to that and this is the one which will come from there. So, if one look at this particular expression, there are so many terms which are involved in this process.

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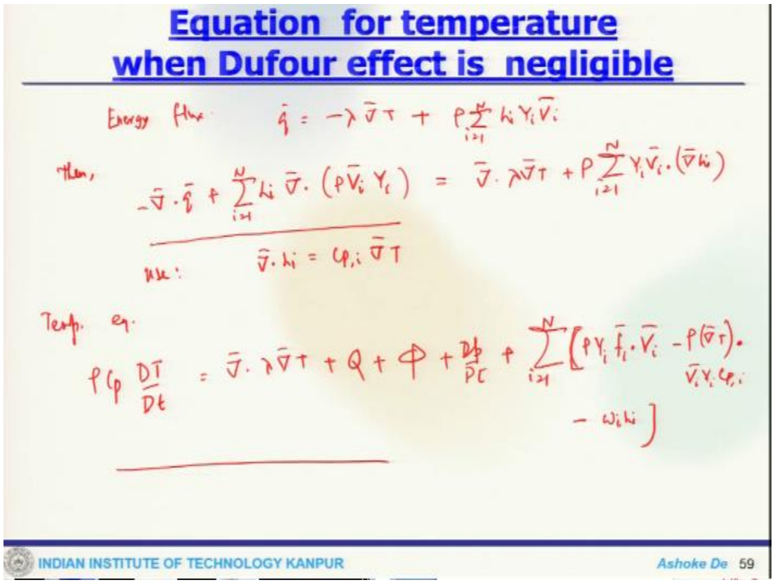

Equation for temperature when Dufour effect is negligible

Energy flux $\bar{q} = -\lambda\bar{\nabla}T + \rho\sum_{i=1}^{N} h_i Y_i \bar{V}_i$

then, $-\bar{\nabla}\cdot\bar{q} + \sum_{i=1}^{N} h_i \bar{\nabla}\cdot(\rho\bar{V}_i Y_i) = \bar{\nabla}\cdot\lambda\bar{\nabla}T + \rho\sum_{i=1}^{N} Y_i\bar{V}_i\cdot(\bar{\nabla}h_i)$

use: $\bar{\nabla}\cdot h_i = C_{p,i}\bar{\nabla}T$

Temp. eq.

$\rho C_p \frac{DT}{Dt} = \bar{\nabla}\cdot\lambda\bar{\nabla}T + Q + \Phi + \frac{Dp}{Dt} + \sum_{i=1}^{N}\left[\rho Y_i \bar{f}_i\cdot\bar{V}_i - \rho(\bar{\nabla}T)\cdot\bar{V}_i Y_i C_{p,i} - \omega_i h_i\right]$

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Now we can see when the Dufour effect is negligible our energy flux can be written

$$\bar{q} = -\lambda\bar{\nabla}T + \rho\sum_{i=1}^{N} h_i Y_i \bar{V}_i$$

So, then one can write

$$-\bar{\nabla}\bar{q} + \sum_{i=1}^{N} h_i\bar{\nabla}(\rho Y_i\bar{V}_i) = \bar{\nabla}\lambda\bar{\nabla}T + \rho\sum_{i=1}^{N} Y_i\bar{V}_i\,(\bar{\nabla}h_i)$$

$$\rho C_p\frac{DT}{Dt} = \bar{\nabla}\lambda\bar{\nabla}T + Q + \Phi + \frac{Dp}{D\tau} + \sum_{i=1}^{N}\rho Y_i\overrightarrow{f_i}\overrightarrow{V_i} - \rho\,(\bar{\nabla}\tau)Y_i\bar{V}_i C_{p,i} - \omega_i h_i$$

then the temperature equation becomes

$$\rho C_p \frac{DT}{Dt} = \overline{\nabla}\lambda\overline{\nabla}T + Q + \Phi + \frac{Dp}{D\tau} + \sum_{i=1}^{N} \rho Y_i \vec{f_i}\vec{V_i} - \rho\;(\overline{\nabla}\tau)Y_i\overline{V_i}C_{p,i} - \omega_i h_i$$

Now if you look at the book of course the temperature equation would be slightly different because some assumption one specific it or not. So, that is pretty much give you an idea, different form that the energy equation can be presented one is total energy, internal energy or enthalpy or temperature.

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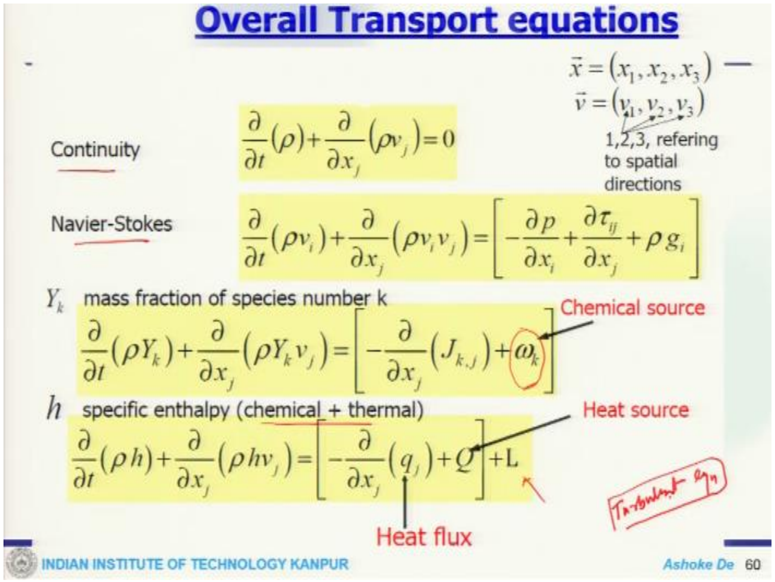

Overall Transport equations

$\vec{x} = (x_1, x_2, x_3)$

$\vec{v} = (v_1, v_2, v_3)$

1,2,3, refering to spatial directions

Continuity $\quad \frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_j}(\rho v_j) = 0$

Navier-Stokes $\quad \frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_j}(\rho v_i v_j) = \left[-\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i \right]$

Y_k mass fraction of species number k

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_j}(\rho Y_k v_j) = \left[-\frac{\partial}{\partial x_j}(J_{k,j}) + \omega_k \right]$$

Chemical source

h specific enthalpy (chemical + thermal)

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_j}(\rho h v_j) = \left[-\frac{\partial}{\partial x_j}(q_j) + Q \right] + \mathrm{L}$$

Heat source

Heat flux

Turbulent eqn

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Now, if I just sort of put the things back together, what is important here to look at is the basic governing equation that one has to have is continuity, this would be like this, the momentum then you have an individual mass fraction and of species where this is the chemical source term and that will tell you whether the species production is there or distraction is there So, that will come from that then we have specific enthalpy, which is a total of chemical plus thermal. So, this is the heat flux term is a heat source and any other source term.

So, that is pretty much taken into account these are my basic governing equation that required for my reacting system. Now, on top of that, what do you need, when it is turbulent, you need the turbulent equation, turbulent equation if it is RANS based equation, then you require RANS based equations, RANS based turbulence model or if it is a list then you require a list based modeling approach and that we see once we move along with our discussion.

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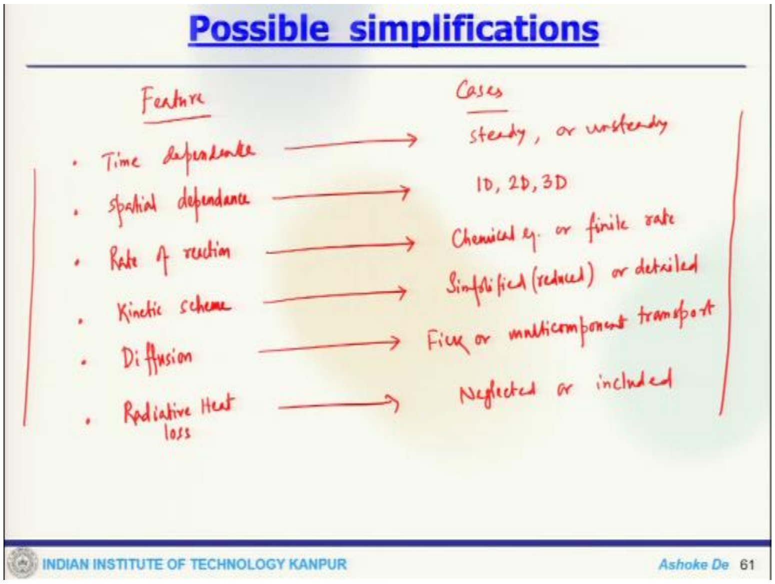

Possible simplifications

Feature		Cases
Time dependence	→	steady, or unsteady
Spatial dependance	→	1D, 2D, 3D
Rate of reaction	→	Chemical eq. or finite rate
Kinetic scheme	→	Simplified (reduced) or detailed
Diffusion	→	Fick or multicomponent transport
Radiative Heat loss	→	Neglected or included

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So, one can do some simplifications here let us say we can categorize like what are the feature and the cases we can simplify accordingly. Let us say if it is time-dependent or dependent, then one can make steady or unsteady. So, these are the possibilities time dependence then you can have spatial dependence which will give you whether it is 1D, 2D, or 3D then depending on the rate of reaction. So, you could have chemical equilibrium or effect of finite rate chemistry, then you can have a kinetic scheme which could be simplified or rather reduced or detailed.

Then you can have diffusion which will be either Fick's law or multi-component transport and finally if you have radiative heat loss this can be either neglected in most of the cases or included. So, you can have certain features and accordingly, you can simplify the cases. So that is why it allows you to do some sort of possible these things.

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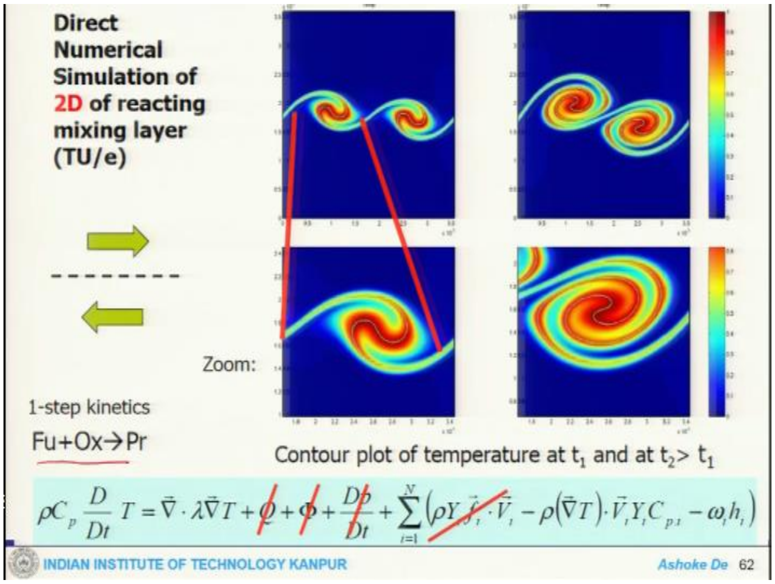

Direct Numerical Simulation of 2D of reacting mixing layer (TU/e)

1-step kinetics

Fu+Ox→Pr

Contour plot of temperature at t_1 and at $t_2 > t_1$

$$\rho C_p \frac{D}{Dt} T = \vec{\nabla}\cdot\lambda\vec{\nabla} T + \cancel{Q} + \cancel{\Phi} + \cancel{\frac{Dp}{Dt}} + \sum_{i=1}^{N}\left(\cancel{\rho Y_i \vec{f}_i \cdot \vec{V}_i} - \rho\left(\vec{\nabla} T\right)\cdot\vec{V}_i Y_i C_{p,i} - \omega_i h_i\right)$$

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Now, this is an image of the reacting mixing layer. This is temperature control. You can see the reaction zone and all these things due to the vertexes and these are the zoomed-in pattern of that. Here the kinetics is simplified because we have fuel plus oxidizer to the product. And the possible simplification for the temperature is that we do not have the effect of Q viscous dissipation, pressure radian these so it says simplified temperature equation which is one can solve this does not give you an idea that how you can simplify it.

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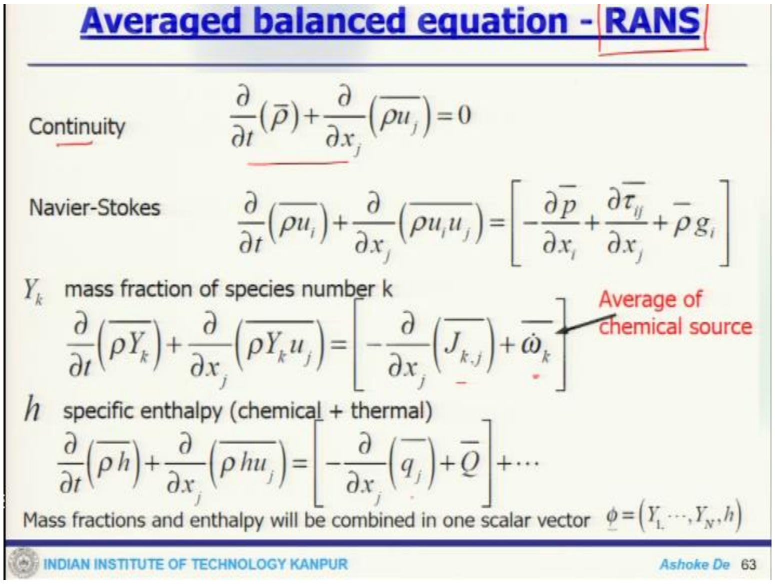

Averaged balanced equation - RANS

Continuity $$\frac{\partial}{\partial t}(\bar{\rho}) + \frac{\partial}{\partial x_j}\left(\overline{\rho u_j}\right) = 0$$

Navier-Stokes $$\frac{\partial}{\partial t}\left(\overline{\rho u_i}\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho u_i u_j}\right) = \left[-\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \overline{\tau_{ij}}}{\partial x_j} + \bar{\rho} g_i\right]$$

Y_k mass fraction of species number k

$$\frac{\partial}{\partial t}\left(\overline{\rho Y_k}\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho Y_k u_j}\right) = \left[-\frac{\partial}{\partial x_j}\left(\overline{J_{k,j}}\right) + \overline{\dot{\omega}_k}\right]$$

Average of chemical source

h specific enthalpy (chemical + thermal)

$$\frac{\partial}{\partial t}\left(\overline{\rho h}\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho h u_j}\right) = \left[-\frac{\partial}{\partial x_j}\left(\overline{q_j}\right) + \overline{Q}\right] + \cdots$$

Mass fractions and enthalpy will be combined in one scalar vector $\underline{\phi} = \left(Y_1, \cdots, Y_N, h\right)$

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Now, we looked at the set of governing equations straight away, since our discussion is primarily on turbulence combustion, we start looking at the system, when we go to RANS based approach that means, when you go to RANS based approach, this would be evaluated equation.

So, the average equation, the balanced equation, continued to look like this, these are Reynolds averaging or the Reynolds average equation Navier stokes will become like that.

And you get then shear stress term system which will also contribute to the radio viscosity species mass fraction equation also will have a diffusion flux and this is an average source term and specific enthalpy we also have the heat flux and the other source term. Now, this would be mass fraction should be sort of a scalar vector.

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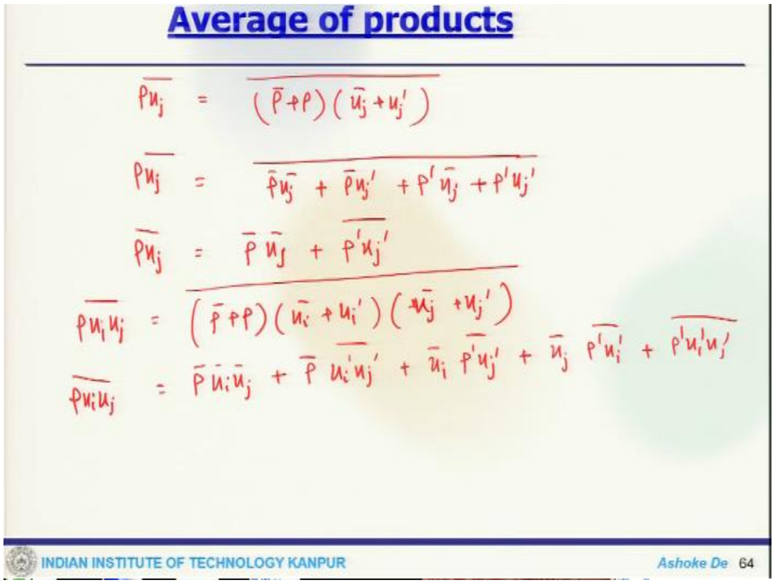

Average of products

$$\overline{\rho u_j} = \overline{(\bar{\rho}+\rho')(\bar{u}_j+u_j')}$$

$$\overline{\rho u_j} = \overline{\bar{\rho}\bar{u}_j + \bar{\rho}u_j' + \rho'\bar{u}_j + \rho'u_j'}$$

$$\overline{\rho u_j} = \bar{\rho}\bar{u}_j + \overline{\rho'u_j'}$$

$$\overline{\rho u_i u_j} = \overline{(\bar{\rho}+\rho')(\bar{u}_i+u_i')(\bar{u}_j+u_j')}$$

$$\overline{\rho u_i u_j} = \bar{\rho}\bar{u}_i\bar{u}_j + \bar{\rho}\,\overline{u_i'u_j'} + \bar{u}_i\,\overline{\rho'u_j'} + \bar{u}_j\,\overline{\rho'u_i'} + \overline{\rho'u_i'u_j'}$$

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Now there is an average of these products. It should be

$$\rho\bar{u}_j = \overline{(\bar{\rho}+\rho)(\bar{u}_j+u_j')}$$

$$\rho\bar{u}_j = \overline{\bar{\rho}\bar{u}_j + \bar{\rho}u_j' + \rho'\bar{u}_j' + \rho'u_j' \ )}$$

So, one can write.

$$\rho\bar{u}_j = \bar{\rho}\bar{u}_j + \overline{\rho'u_j'}$$

$$\rho\overline{u_i u_j} = \overline{(\bar{\rho}+\rho)(\bar{u}_i+u_i')(\bar{u}_j+u_j')}$$

So that is using the averaging property for RANS based framework. So these would become like

$$\rho\overline{u_i u_j} = \bar{\rho}\bar{u}_i\bar{u}_j + \bar{\rho}\overline{u_i'u_j'} + \bar{u}_i\overline{\rho'u_i'} + \overline{\rho'u_i'u_j'}$$

Now, the terms which continue the density fluctuations do not appear in the alternative approach. So that is why if you use the density average reinstituted average that would not appear. So that is all we will look at it, how you can eliminate those term using fluctuations of the density fluctuation. So stop here today, and we will continue the discussion at the next level.