


Fundamentals of Combustion
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Lecture - 24
Governing Equations for Reacting Flow - Part 1
Continuity, Momentum and Species Conservation Equations


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Governing Equations




Governing equations are partial differential equations representing the conservations of mass, momentum, species and energy in a infinitesimal control volume.

For several practical problems, these equations are arrived at by invoking the continuum (macroscopic) approach. Here, the control volume where conservation is sought is much smaller than the entire domain, but much larger than the mean free path of molecules.

In a control volume, several molecules enter and exit through control surfaces, transporting mass, momentum and energy into and out of it. As a result, a change of these quantities may occur within the control volume as a function of time.

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The next topic is the governing equations for reacting flow; the governing equations of reacting flow are conservation equations basically; so, they will conserve several quantities. They conserve mass, mass of the mixture, mass of individual species, then momentum of the mixture; the species; individual species is conserved, then energy is conserved.

So, these are conservation equations; so we have to conserve in this reactive flow or in any combustion environment, we have to conserve mass, momentums, species and energy.

So, we use partial differential equations to write the conservation of these quantities and we actually write this the equation and integrate over assuming a very small control volume, infinitesimal control volume is taken and in this the conservation is made and partial differential equations are derived.

So, main assumption what we make here is the continuum approach; the continuum approach or which is called macroscopic approach. So, what is macroscopic approach? See there are molecules of several gases present in the reactive system.

If you want to trace each and every molecule and understand where it is located, what is the velocity with which it moves etcetera; it is not possible for us to analyze anything. So, we are not interested in the molecule level values or quantities, we are interested only in the average effect of these molecules; so that approach is called macroscopic approach. So, what we allow here is we will take several molecules and only see the average effort of these molecules on several measurable, observable and say calculatable properties. So, like pressure, temperature, enthalpy everything; we can get this, but these are all not due to an individual molecule, we cannot go to the molecule level; it is only an action of several molecules; average effect of several molecules put together.

So, we choose a control volume and do the conservation of these. Now, this control volume where the conservation is done is smaller than the entire domain. For example, if we take this room, big room; we will only consider here say $1\text{ cm} \times 1\text{ cm} \times 1\text{ cm}$ control volume. So, it is much more than this room size, but this 1 cm is much larger than the mean free path of a particular molecule.

So, molecule before hitting with another molecule; they travel a particular distance called mean free path; that length scale is much smaller than the control volume what you take into account.

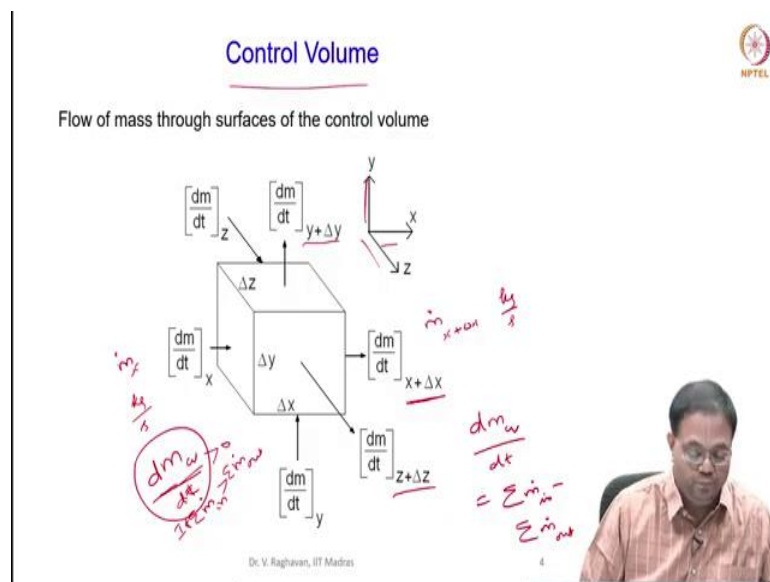
So, just giving some examples; so in the macroscopic approach we do not go into molecule level details and we can use classical thermodynamic approaches here for the solving our problems.

Now, in a control volume; several molecules enter and exit through controls surfaces. So, control volume, you can actually take a Cartesian control volume.

So, Δx , Δy and Δz , Cartesian control volume say cuboid and so six faces are there through which molecules can enter and leave so, those surfaces are called control surfaces.

Now, when the molecule enter; they can transport mass, momentum, energy in and out of it. So, as a result of these transport, there will be changes within the control volume, there will be changes in these quantities as a function of time. So, this is the principle what use for deriving the conservation equations.

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A control volume; so, you can see that control volume is shown here; as I told you we have taken the Cartesian coordinate. So, this is x direction here; x direction is horizontal direction, vertical direction is y direction here and z direction is the mutually perpendicular direction.

So, there are 6 faces; let us take the x direction for example, in this face, perpendicular to this face some mass is entering, so some this is $[dm/dt]_x$, let us say first some mass is entering, this is \dot{m} and at the station of x it is entering.

So, we say \dot{m}_x kg/s; that is the mass entering here and the mass leaving at the station $x+\Delta x$ is given by $[dm/dt]_{x+\Delta x}$, this is written like this; So, this is also kg/s; so this is in the

x direction. Similarly, we can write for the mass entering through the bottom face is $[dm/dt]_y$ and that leaving the top surface is $[dm/dt]_{y+\Delta y}$.

Similarly, the z direction $[dm/dt]_z$ and $[dm/dt]_{z+\Delta z}$. Now, if the net mass entering, that is $[dm/dt]_x$, $[dm/dt]_y$ and $[dm/dt]_z$ that is same as the net mass leaving $[dm/dt]_{x+\Delta x}$, $[dm/dt]_{y+\Delta y}$, and $[dm/dt]_{z+\Delta z}$. Then, there will be no accumulation of mass in this. But if the net incoming mass is higher than the outgoing mass, then mass will accumulate with time.

So, if you say dm_{cv}/dt of control volume, this control volume; the rate of change of mass of control volume with time, this will be greater than 0; if say $\sum \dot{m}_{in}$ is greater than $\sum \dot{m}_{out}$ or we can simply write $dm_{cv}/dt = \sum \dot{m}_{in} - \sum \dot{m}_{out}$, so this is simple mass conservation.


So, in this form we are writing, but when you translate this and write the entire equation, you will end up in a partial differential equation. So, this is about mass. Now, instead of mass; mass multiplied by velocity that is momentum can enter through these surfaces.

Similarly, momentum can change within the control volume, similarly energy can enter. So, this mass into a specific energy that can enter and leave through other surfaces so that that net energy of the control volume can increase or decrease based upon the entering and leaving quantities.

So, this is the control volume approach where we seek the flow through surfaces of control volume in and out and try to write the conservation equation for the particular quantity. So, mass, momentum, energy, species etcetera.

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Species Conservation



Conservation of each species (say species A) in the multicomponent mixture is governed by,


$$\frac{\partial (\rho Y_A)}{\partial t} + \nabla \cdot [\rho Y_A (\vec{V} + \vec{v}_{A,diff})] = \dot{\omega}_A''$$

$\vec{v}_A = \vec{V} + \vec{v}_{A,diff}$ $\dot{\omega}_A''$ (kg/m³·s) $\rho Y_A = \rho_A$

Rate of mass of species A accumulated in the control volume plus the net mass efflux (outgoing flux – incoming flux) of species A through the surfaces of the control volume is equal to the net rate of its production (or destruction), denoted by the term in the right-hand side ($\dot{\omega}_A''$), which has units of kg/m³·s. The net mass efflux of species A includes the fluxes due to convection (\vec{V}) as well as diffusion ($\vec{v}_{A,diff}$).

$\sum_{A=1}^N \dot{\omega}_A'' = 0$

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Now, let us first see the species conservation. So, detailed derivations are not given here, but we will understand physically the terms involved. So, for example, conservation of species; one of the species, let us take we have to actually do several species; for example, if N number of species are present in a mixture at least we have to conserve N-1 species.

So, let us take a particular species say species A and try to write the conservation equation for this species. So, this is written as partial derivative of the quantity ρY_A ; ρ is the mixture density, Y_A is the mass fraction of the species, this is the mass of this species.

$$\frac{\partial}{\partial t} (\rho Y_A) + \nabla \cdot [\rho Y_A (\vec{V} + \vec{v}_{A,diff})] = \dot{\omega}_A'''$$

So, ρY_A will be equal to m_A , mass of the species A. The rate of change of mass of the species A with time. So that is written here, per unit volume; this is actually written per unit volume basically. So, this is actually not $\rho_A \times V$, if you put you get m_A .

So, now this is written per unit volume. So, rate of change of mass of species A, per unit volume is this term. Now, that is equal to that plus the convection; when the species comes in, it comes in with this its flux. So we know this.

So, $\rho_{AV_A} = \rho V Y_A - \rho D_{A,m} \times dY_A/dx$, in the x direction let us take. So, this is the net mass flow rate of A, per unit area of cross section through a particular face.

So, when you try to do this and take the sum of all, you get this term. So, due to convection of the species through all the faces. What is the net mass convected away - the net mass coming in, that term is the second term here.

This convection actually involves the species velocities. What is species velocity of A? The bulk velocity + diffusion velocity of A. So, this species velocity, this term here represents the species velocity vector of A.

So, with its own velocity it is convected out of the control volume through some surfaces and convected in through some surfaces. The outgoing flux that is mass flux is what? Mass flow rate/cross sectional area - incoming that net mass efflux; that is outgoing mass flow rate/unit area - incoming mass flow rate/unit area that term is this second term here is called convective term; so this term is called convective term.

Basically, in this particular case it also includes a diffusion. The convective term also includes these actually. Why I say it is convective term, because it involves this species velocity, but species velocity itself has two components, the bulk convection of the mixture and the diffusion of the particular species into this mixture.

So, the rate of change of the mass of the species per unit volume plus the net mass efflux of the species through the control volume will be equal to the rate of production or consumption of the species; this can be positive or negative; this $\dot{\omega}'''$.

So, this has the unit of $\text{kg/m}^3\text{s}$ and this is actually written as some coefficient into concentration of species A, concentration of species B etcetera. Some reaction rate, net reaction rate; it cannot be one equation, it may be several. So, what we saw in the previous lecture; $d[\text{O}_2]/dt$ involving say four reactions, three reactions and several forward and backward reactions etcetera.

So, this is a net rate of production or consumption of species A; so that can be written in this $\text{kg/m}^3\text{s}$. So, the conservation statement is rate of mass of species A accumulated in the control volume.

So, please add per unit volume plus the net mass efflux; that is outgoing flux, outgoing flow rate/unit area is called out going flux - incoming flow rate/unit area of species A, through the surfaces of the control volume is equal to the net rate of its production or destruction, denoted by the term in the right hand side. $\dot{\omega}_A'''$.

So, triple dash actually represents per m^3 ; so every term is per m^3 per unit volume. So, the net mass efflux of species A is convection term basically because it involves convection of the species velocity A, but this species velocities is calculated using the bulk velocity; mixture convection velocity + the diffusion velocity, so this is the species conservation.

So, we have to understand that N-1, see if N multicomponent species are present, N-1 equations are going to be solved like this with non-linear source terms. So, this is a non-linear term; this term is the non-linear source; $A \times \exp(-E_a/R_u T)$ so that the exponential dependence on temperature is present. That becomes a highly non-linear source.

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Continuity Equation

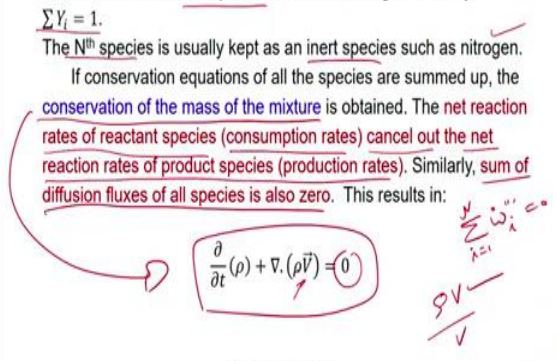

In a multicomponent mixture with N components, $(N-1)$ species conservation equations are solved to obtain their mass fractions. Mass fraction of the N^{th} species is obtained using the identity, $\sum Y_i = 1$.

The N^{th} species is usually kept as an inert species such as nitrogen.

If conservation equations of all the species are summed up, the conservation of the mass of the mixture is obtained. The net reaction rates of reactant species (consumption rates) cancel out the net reaction rates of product species (production rates). Similarly, sum of diffusion fluxes of all species is also zero. This results in:

$$\frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho \vec{V}) = 0$$

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So, as I told you when there are N components; $N-1$ species conservation equations are used. So, that is why we use that steady state approximation or partial equilibrium approach to reduce the number of species, the number of species to be solved using a partial differential equation. So, this is a partial differential equation, here partial differential equation is written in vector form.

Now the N^{th} species is calculated by using this identity, so $\sum Y_i = 1$. So, the mass fraction of N^{th} species is calculated using this identity. The N^{th} species normally will be kept as inert species such as nitrogen. Nitrogen will not react much. So, that will be the N^{th} species so we need not solve for the transport equation, just calculate using the identity.

Now, this equation is for one particular species say A . Now, add for all the species. Write these equations for all the N species and add them, you will get the conservation of mass of mixture. Do you understand?

So, conservation of the mass of each species is summed up for all the species will give the conservation of mass of the mixture. So, let us say, take the right hand side now, what happens to the right hand side?

There is a term called $\dot{\omega}_A'''$. Now, you sigma this term from 1 to N , so this will become 0. How? because the net reaction rate of the reactant species which are consumption, they are negative values cancel out the net reaction rate of the product species, production rate positive.

So, they will cancel each other so that you will get the $\sum \dot{\omega}_i''' = 0$, $i = 1$ to N . So, that is going to eliminate the source term, so you will see that there is no source term in the conservation of mass of mixture.


Now, if you take the diffusion fluxes, so we are now having only this velocity here, but what about the species velocities due to diffusion. So, v_A , diffusion velocities. What happens to that? The diffusion fluxes of all the species is also going to be 0; sum of the diffusion fluxes of all the species when summed up they are going to 0. So, that will eliminate the diffusion velocity appearing in this.

So, we get a simple equation for conservation of mass of the mixture which is nothing, but the partial derivative of ρV , that is the rate of the accumulation of the mixture mass inside the control volume.

$$\frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho \vec{V}) = 0$$

So, ρV , per unit volume is $\rho V/V$ is ρ . So, that the rate of change of mass of the mixture; ρV (the mass of the mixture)/ unit volume + the net efflux of the mixture which is transported out of the control volume/unit area - the mass which is coming into the control volume.

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Continuity Equation

Continuity equation represents the overall mass conservation.


Mass of the multicomponent mixture accumulated within the control volume plus the net efflux of the mixture mass through the surfaces of the control volume is equal to zero.

For reacting flows observed in burners and stoves, the velocities involved are quite low and the flow is incompressible in nature.

In several applications involving flow processes, the total pressure remains almost a constant. In these scenarios, the density of the mixture varies due to variations in temperature and composition of the mixture.

$\frac{\partial \rho}{\partial t}$

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So, continuity equation represents the overall mass conservation; mass of the multi component mixture accumulated within the control volume, the transient term, the time dependent term + the net efflux, that is the outgoing mass flux - incoming mass flux of the mixture. So, net efflux of the mixture mass through the surfaces of the control volume is equal to 0.

That is the simple continuity equation what we have here; continuity equation or conservation of mass, we get mass of the mixture. Now, some points to ponder; for reacting flows like observed in burners and stoves, the velocities are very low; we do not have very high velocities.


So, even if you have a turbulent flow, velocities are not very high. So, mach number will be very low say less than 0.3; so the flow is assumed to be incompressible. See why I am saying this here because if you go back, you have this term here, the rate of change of mixture density with time.

So, normally when the velocity is very low and the flow is incompressible in nature, people will think that the density will not change at all; density is constant.

So, incompressible flow, density is constant; that will be the thinking, but here this term is important, we cannot neglect this term because even though the flow is incompressible; that temperature dependence is there and also the species will be changing. The concentration of the species in a particular location and the temperature at a particular location will be changing.

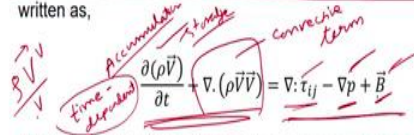
Similarly, with time also the concentration and the temperature will vary. So, rate of change of mixture density with this time is due to the change of temperature and composition of the mixture. That is even though the flow is incompressible, density is not constant; density will vary as a function of temperature and composition of the mixture; so that we have to understand.

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Momentum Conservation


Momentum conservation follows the **Newton's second law of motion**. For fluids, it is stated as the **rate of change of momentum in a control volume is equal to sum of all forces acting on the control volume**. It is written as,



$$\frac{\partial(\rho \vec{V})}{\partial t} + \nabla \cdot (\rho \vec{V} \vec{V}) = \nabla \cdot \tau_{ij} - \nabla p + \vec{B}$$

First term in the left-hand side represents the **rate of change of momentum per unit volume**, the **second term** in the left-hand side is the **convective term**, $\nabla \cdot \tau_{ij}$ is the **gradient of the stress tensor** (τ_{ij}), which includes normal and shear stresses at the control surfaces, ∇p is the **pressure gradient** and the last term in the right-hand side, \vec{B} is the **body force vector**.

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So, next equation is the momentum conservation equation. So, momentum conservation equation actually follows Newton's second law of motion. For the fluid, we can say the

rate of change of momentum in a control volume is equal to the sum of all forces acting on the control volume.

$$\frac{\partial(\rho\vec{V})}{\partial t} + \nabla \cdot (\rho\vec{V}\vec{V}) = \nabla : \tau_{ij} - \nabla p + \vec{B}$$

So, that is the simple statement what we can make about this. Now, what is in the left hand side of this equation? This is the momentum equation, again compactly written in the vector form. So, now see that the first term we have discussed a lot; this is the momentum, the rate of accumulation of momentum of the mixture in the control volume; so $\rho\vec{V}$; vector that is the moment in a particular direction.

So, this is a vector; so you can dissolve it into three directions, this divided by the volume. So, rate of change of momentum. So, this multiplies volume divided by volume; so this will be the momentum, $\rho\vec{V}\vec{V}$ that is momentum per unit volume.

So, rate of change of momentum per unit volume in the control volume plus this is the convective term. Again, the net efflux of momentum; so $\rho\vec{V}\vec{V}$ across the surface only this happened. So, $\rho\vec{V}\vec{V}$ is the mass flow rate of the mixture into its velocity \vec{V} , that will be the momentum.

So, you can again dissolve into three directions so $\rho\vec{V}\vec{V}$. So, when you again divide it by volume etcetera or write in gradient terms etcetera, you will see that this is going to be the efflux of momentum; that is the outgoing momentum flux - incoming momentum flux across the control surfaces in the control volume; so, convective term.

So, this is the storage term or accumulation term; again, lot of nomenclatures are there. Its accumulation or we can also say time dependent. So, time dependent term or accumulation term or storage term; anything can be used for the first term where within the control volume, there is a rate of change of the momentum as a function of time.

So, this is the left hand side; rate of change of momentum in the control volume and through the control volume surfaces, across the control surfaces. So, net rate of change of momentum is in the left hand side. The right hand side, forces first term is the $\nabla : \tau$; this is the gradient of stress tensor, stress tensor will show you in next slide.

So, this is gradient of stress tensor; so this will involve the normal stresses and shear stresses acting on the control surfaces and these are the forces due to the viscosity of the fluid, due to the viscosity of the fluid these stresses are appearing.


So, due to pressure; the pressure gradient, pressure forces will be added that is represented by the pressure gradient here and some body forces that can be absorbed in

this term \vec{B} . So, body force vector is the B vector. So, these are all the force terms surface force, pressure force, body force; this is volumetric.

So, surface forces are due to viscosity effects; both normal and shear stresses are included here, pressure-based forces and the body forces. So, rate of change of momentum in the control volume and across the surfaces of the control volume; net rate of change of momentum is equal to the forces acting on the control volume surfaces and within the control volume, body force is a volumetric term.

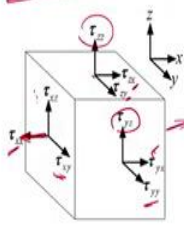
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Momentum Conservation



\vec{B} is expressed as, $\vec{B} = \rho \sum_{k=1}^N Y_k \vec{f}_k$

Here, \vec{f}_k is the volumetric force per unit mass acting on k^{th} species.
 Stress tensor, shown in the figure, can be written in terms of velocity gradients. In tensor form, it is written as,



$$\tau_{ij} = \left(\mu' - \frac{2}{3}\mu \right) \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

Here, μ is the dynamic viscosity of the mixture and μ' is secondary (or bulk) viscosity.

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Now, the \vec{B} is nothing but the force, see \vec{f}_k is the force, volumetric force per unit mass on a k^{th} species. Similarly, you have to add for all the N species.

$$\vec{B} = \rho \sum_{k=1}^N Y_k \vec{f}_k$$

So, mass fraction of the species into the force acting on the species that summed up into the mixture density will give you the body force this will be added, but this will be negligible actually. So, this actually in several cases it is negligible. So, this is the body force term that can be added, if you want to add you can add it; next stress tensor is like this.

$$\tau_{ij} = \left(\mu' - \frac{2}{3}\mu \right) \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

So, you can see a stress tensor; you have normal stresses, see for example, here τ_{xx} . Similarly, in the opposite also the same pattern will appear. So, this is symmetric in nature. So, normal stresses are τ_{xx} , τ_{yy} and τ_{zz} . The stresses are also acting tangential to the surface.


For example, here τ_{xy} and the τ_{xz} in this plane; so in the top plane τ_{zx} , τ_{zy} they are parallel to the surface; similarly in the other side you get τ_{yz} and τ_{yx} . So, all these contribute to shear stress, the tangential components add to the shear stresses, normal component add to the normal stresses.

Everything can be written in terms of viscosity this is the dynamic viscosity because the stress tensor in a form is written in terms of the gradients of velocities; velocity gradients and viscosity. So, you also use what is called as bulk viscosity or secondary viscosity which is actually negligible in several applications.

So, this is the shear stress and this is the normal stress and so this is actually equal to 1, so $\delta_{ij} = 1$, if $i = j$, or $\delta_{ij} = 0$, if $i \neq j$. So, now this is the stress tensor which is written in terms of gradients of velocities; velocity gradients; u_i , u_j , u_k etcetera are the velocities used here and these are all the directions x_i can be x direction, x_j can be y direction, x_k can be z direction and so on. μ is the dynamic viscosity and μ' is the second viscosity; so this is the viscous term. So, once you know the viscous term, body force term and pressure is known, the entire equation can be formed.

So, this is the entire equation; the forces due to viscous effects, this is the pressure induced forces; pressure gradient, the volumetric body force and this is the stress tensor here.

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Energy Conservation

Energy conservation is stated as *the rate of accumulation of total energy is equal to net efflux of total energy plus 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 $\rho(\vec{V} \cdot \vec{V})/2$. It is written, per kg of the mixture, as,

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

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So, I will stop here. We will continue with the energy conservation in the next class.