

Combustion in Air Breathing Aero Engines
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Lecture - 13
Governing Equations I

Welcome back. As we discussed will talk about governing equations; and these governing equations will essentially described are basically used for describing the entire flow field for any combustion process. So, as we will see that or as we can anticipate that these governing equations comes from basically conservation principles, conservation of mass, conservation of momentum, conservation of scalars, conservation of energy. So, basically all these conservation principles and how generation of something leads to the depletion of that one or generation and depletion of these quantities and how that effects that can couple with the flow field etcetera that will see.

Basically you will see that, that this conservation of mass is essentially is coupling between we will see that will basically involves density and velocity. The conservation of momentum once again involves density, velocity and pressure, because essentially the pressure gradients is the characteristic force here and that will cause acceleration or deceleration in a flow and as well as this the fictional loss due to the presence of viscosity. Then we will see that how species can be advected or a particular species can be advected along with the flow, and how it can defuse a region of high concentration to region of flow concentration and how also it can be generated or depleted because of the source terms which comes from the chemical reaction rates.

And the conservation of this energy that is which will start with a internal energy form and then will go into the enthalpy form and then we can show that we can show that we can allow at a temperature form. And we will also see that how this enthalpy can be transported with the flow then it can be also can be there can be pressure that can affect the enthalpy if the time variation of pressure. And then also there can be like conduction processes, heat conduction processes as well as enthalpy transport due to the different diffusion velocities and also how the enthalpy of formation is essentially get converted into sensible enthalpy through the heat release term inside the energy equation.

So, these governing equations are very, very pivotal and are central to your understanding of the flow processes inside a combustor, because it is using these governing equations we actually plug in our understanding of kinetics or understanding of transport or understanding of convection all these things come into and are basically assembled using these governing equations.

So, with these governing equations of course, when you discretize when you do a discretization and then in a grid you can actually solve using CFD computational fluid dynamic technique to solve the flow inside actual combustor also, either you are doing theory or you are doing experiments or you are doing CFD, you must know the governing equations and understand what each term represents.

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Module 5
Governing Equations

- i. Control volume derivations →
- ii. Conserved scalar formulation
- iii. Reaction sheet formulation ←
- iv. A simplified system & non-dimensional numbers ←

Majority of the material is taken from
i. Combustion Physics by C. K. Law, Cambridge University Press.

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So, first we will do this with do will do this control volume derivations, and then we will also for different things like mass, momentum and energy. We will go to this conserved scalar formulation. And then these two things this reaction sheet formulation and simplified one-dimensional numbers will go into in a latest stage when we will go into look into the actual flames.

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Introduction

- Chemically reacting flow are governed by conservation laws for mass, momentum, energy, and concentration of individual species
- The conservation laws are derived keeping in mind the continuum hypothesis
- The governing equations model the multicomponent, reacting, flow with a set of partial differential equations (PDEs)
- Along with the governing PDEs, constitutive and auxiliary relations are required to form a set of closed equations.
- These equations can be simplified under suitable assumptions

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So, as we said that chemically reacting flows, combustion is of course, very solid example of chemical reacting flow. So, chemically reacting flows are governed by conservation laws for mass, momentum, energy and concentration of individual species. So, the conservation laws are derived keeping in mind the continuum hypothesis of course, you know about the continuum that is when you look in to a small part inside the flow, you will still find density to be uniform. Inside very small part of the flow and it is not happen does not should discrete jumps due to presence of one molecule and then nothing then one molecule. So, it is nothing like that. So, the continuum hypothesis is certainly preserved in these cases. So, one can define density as a continuous variable which is mass per volume.

And then the governing equations model the multi component reacting flow with a set of partial differential equations. So, we will start with integral equations and then will move onto partial differential equations. And along with the governing partial differential equations, the constitutive and auxiliary relations are required to form a set of closed equations. So, the conservation laws that will use that these does not close the problem, this will only give rise to this partial differential equations, but to close this partial equation differential equations, we need this constitutive and auxiliary relations. And of course, as we will see that or this equations will be very complex in their full forms, and will appropriately simplify them under suitable assumptions.

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Control Volume Formulations

Reynolds Transport Theorem (RTT):

Time-rate of change of an extensive property Ψ	=	Time-rate of change of Ψ within a control volume	+ Flow-rate of Ψ across the control surface
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- Extensive fluid property $\Psi = \int_V \psi dV$

$$\frac{\delta \Psi}{\delta t} = \frac{\partial}{\partial t} \int_V \psi dV + \int_S \psi (\mathbf{v} \cdot \mathbf{n}) dS.$$
- Divergence theorem: $\int_S \psi (\mathbf{v} \cdot \mathbf{n}) dS = \int_V (\nabla \cdot \psi \mathbf{v}) dV,$

$$\frac{\delta \Psi}{\delta t} = \int_V \left(\frac{\partial \psi}{\partial t} + \nabla \cdot \psi \mathbf{v} \right) dV.$$

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So, the central theorem that we use for understanding the conservation laws in fluids is the Reynolds transport theorem. Now, this Reynolds transport theorem is very, very central because it allows us to use our knowledge of conservation laws for a system to our control volume. That is to give you an example, suppose this is my control volume, this is red boundaries my control surface and then there is a packet of fluid which is this there is a system which is moving. So, say this packet of fluid I was at this position at time t minus Δt this occupies inside of the control volume at t and then this packet moves out at time t plus Δt .

And what I want to say is that the laws of physics say like Newton's law or the mass conservation that you know is for this packet of fluid which is moving. The mass of it is not changing the momentum of this if there is no external force it is not changing. And this energy, if there is no external in supply of energy or loss of energy that is also not changing, but that is not what we are interested.

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Control Volume Formulations

Reynolds Transport Theorem (RTT):

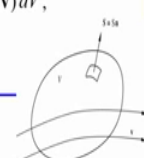
$$\frac{\text{Time-rate of change of an extensive property } \Psi}{\delta t} = \frac{\text{Time-rate of change of } \Psi \text{ within a control volume}}{\delta t} + \frac{\text{Flow-rate of } \Psi \text{ across the control surface}}{\delta t}$$

- Extensive fluid property $\Psi = \int_V \psi dV$

$$\frac{\delta \Psi}{\delta t} = \frac{\partial}{\partial t} \int_V \psi dV + \int_S \psi (\mathbf{v} \cdot \mathbf{n}) dS$$

$$\Psi = \int_V \psi dV$$
- Divergence theorem: $\int_S \psi (\mathbf{v} \cdot \mathbf{n}) dS = \int_V (\nabla \cdot \psi \mathbf{v}) dV$,

$$\frac{\delta \Psi}{\delta t} = \int_V \left(\frac{\partial \psi}{\partial t} + \nabla \cdot \psi \mathbf{v} \right) dV$$



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We are interested in applying this law inside a control volume. Why, because suppose your engine your engine is actually a control volume all right. So, you are not interested in the mass of packet of mass that goes in at different state and that goes out. We are interested in what happens inside this control volume. So, first we need to understand the law that will translate the conservation laws from the system to the control volume. So, what does it say, it says that of course, we can go this in details, but this is not our fluid mechanic class or thermodynamics class. So, we will just leave it leave it here itself.

It says that the time rate of change of an extensive property Ψ . Please note that this is a time rate of change of the extensive property Ψ which is within a system is essentially equal to the time rate of change of Ψ within the control volume, and the flow rate of Ψ across the control surface. So, of course, when you are moving a packet of this fluid, there is no inlet or outlet, but in this control volume that you are defined in this thing, there is continuous inlet and this continuous outlet. So, it says that it is a time rate of change of Ψ that is happening inside this control volume and that amount of Ψ that comes in and that amount of Ψ that gone out, the difference between them, so that also you need to take care of. So that is the basic essence of Reynolds transport theorem.

And here we use this extensive fluid property Ψ capital Ψ is nothing but capital Ψ is equal to integral small ψ dV that is so this Ψ is equal to integral ψ dV where V is the volume of the control volume in this when it is capital V in this manner.

But you have to be careful sometimes we will use v as velocity also. So, please be careful with that. So, this says that this $\frac{d\psi}{dt}$ that is the total derivative of this property ψ following it in a system sense is essential is equal to $\frac{d\psi}{dt} \int_{CV} \rho \, dV$ that is integral over the control volume plus the integral over the surface ψ times $v \cdot n \, dA$, where the n is essentially the surface normal. So, this part $v \cdot n \, dA$ basically characterizes the mass flow rate that is happening, and also this multiply with ψ gives us the flow rate of the property ψ that is happening.

If this is a moving control volume then this essentially becomes v relative. So, that is velocity the actual velocity minus the velocity of the control volume. So, this is the Reynolds transport theorem. And then using this which is defined entire surface, you can convert this surface integral into a volume integral using Gauss divergence theorem, so which is given this. So, once you have converted it, you see that that basically this is also an in volume integral, this is also volume integral. So, you can write that using this you can write that $\frac{d\psi}{dt}$ is equal to $\int_{CV} \frac{d\psi}{dt} \rho \, dV$ plus divergence of ψv integral over the entire control form.

So, this is the basic formula for going from a system representation to a control volume representation. This is for a system that is a rate of change of property ψ for when you are following that packet when you are following that system by system we mean that there which does not through which there is no mass flow rate that is happening. So, when you are following the packet of fluid the rate of change of that over ψ on that packet is given by this, but when that packet enters passes to a control volume, this is given by this volume integral.

So, this is how you basically connect. So, essentially this is the rate of change of ψ of the connection happens that this is the rate of change of ψ happening inside the packet of fluid when it is inside in the inside the control volume and that must be equal to the rate of change of the property ψ . When it is within the control volume plus the flow rate of ψ that is happening across the control surface, so this is how you connect. So, integral of v is nothing but this $\frac{d\psi}{dt} \int_{CV} \rho \, dV$ plus divergence of $\rho \psi v$.

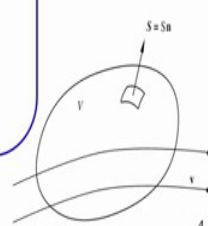
So, now this psi is essentially a generalized property, but we can use this for any property. And we will use this to basically derive the basically change the representation of psi, sometimes we will consider psi as mass, sometimes will consider psi as momentum, sometimes will consider psi as a mass of certain species certain kind, then sometimes will consider psi as a total energy. And by changing this representation of psi, as we see did before also for the for deriving the transport properties, we will arrive at the conservation loss is essentially mass, momentum, species and energy

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Control Volume Formulations

Definitions of velocities

- v_i velocity of i^{th} species
- v mass-weighted bulk fluid velocity
 $\sum \rho_i v_i = \rho v$
- V_i molecular diffusion velocity $V_i = v_i - v$
 Consequently, $\sum \rho_i V_i = \sum \rho_i v_i - \rho v = 0$
- $Y_i = \rho_i / \rho$; $v = \sum Y_i v_i$; $\sum Y_i V_i = 0$
- Y_i - mass fraction

$$\sum \rho_i \vec{v}_i = \sum \rho_i \vec{v}_i - \rho \vec{v} = 0$$


So, now first we need to understand that this we need to understand the concepts of the definitions of the velocities because here as we know combustion the difference between combustion and other an fluid mechanics because here we not only involve reactions, but we also involve multiple species, it is not one kind of a fluid. So, so v_i is the velocity of the i -th species, this small v_i and this average this small v is the mass-weighted bulk fluid velocity. So, this is these v is essentially the velocity that we have familiar with. So, this is the mass-weighted bulk fluid velocity with which interfere is moving v_i is the velocity the average of the of the i -th species with is a velocity with which the i -th species is moving.

So, summation $\rho_i v_i$ is equal to ρv . So, $\rho_i v_i$ is nothing, but the ρ_i is nothing but the partial density and we will see that how ρ_i is defined is nothing but y_i , there is a mass fraction is essentially ρ_i divided by the divided by ρ . Partial density means

the mass of the species i divided by the total volume; velocity density is the mass of the full thing of the entire all the components divided by total volume. Where is this v_i is the molecular diffusion velocity which is nothing but capital which is this represent by capital V_i is nothing, but this velocity if the i -th species minus the bulk velocity mass-weighted bulk velocity. So, consequently it can be shown that summation ρ_i capital V_i is equal to essentially $\rho_i v_i$ summation $\rho_i v_i$ minus ρv .

Why this is so because if we consider this thing summation $i \rho_i v_i$ vector is equal to if you start with let us start with v_i vector is equal to v_i vector minus v vector. So, let us multiply both sides with ρ_i ρ_i ρ_i and then you sum over it, sum it, sum it. So, then what we will get is that summation $\rho_i v_i$ vector is equal to this stage as is summation $\rho_i v_i$ vector minus when you this does not contain i . So, we only sum over ρ_i , summation ρ_i is nothing but ρ . So, this is equal to ρv , but as we have seen here that summation $\rho_i v_i$ is equal to ρv . So, this two are essentially equal and this becomes is equals to 0.

So, also this v_i is so using that using this formula and this formula, we can find out the actual v velocity is essentially nothing but summation $\rho_i y_i v_i$, y_i is the mass fraction. And also we can show that using this because this equals to 0 which is divide both side by ρ and you get both side is dividing by ρ , you get y_i and you get summation $y_i v_i$ is nothing but equal to 0. So, these are some of the important definitions of velocity is that we will use.

Now, please understand the difference between this velocity this velocities this is the velocity of the i -th species this is the mass-weighted bulk fluid velocity and this v_i is the molecular diffusion velocity which is nothing but difference between the velocity of the i -th species and the bulk weight velocity. So, that is the molecular diffusion velocity and none of this will be actually equal to 0 in a given scenario in a particular case inside a say flame or something.

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The slide features a green header with the title "Conservation of Total Mass". Below the header is a white text box with a blue border containing the text: "Following RTT, the rate of change of mass is equal to sum of change of mass in C.V. and flow of mass across the control surface". Below the text box, the following equations are written in red ink:

$$\frac{\delta \Psi}{\delta t} = \int_V \left[\frac{\partial \psi}{\partial t} + \nabla \cdot (\psi \cdot \vec{v}) \right] dV$$
$$\Psi = \int \psi dV$$
$$m = \int \rho dV$$

A small number "5" is located in the bottom right corner of the slide.

Now, how to give: now also if you remember now you consider that we derive this formula that is $\frac{d \psi}{dt}$ rate of change of this property ψ capital ψ and the system which is inside just inside the control volume is given by $\int_V \frac{\partial \psi}{\partial t} + \nabla \cdot (\psi \cdot \vec{v}) dV$ plus divergence of $\psi \cdot \vec{v}$ vector, this \vec{v} is a bulk fluid velocity dV . This V is volume. So, this is what we have got.

Now so the rate of from Reynolds transport, Reynolds transport theorem we can say that the rate of change of mass just by why changing with from the property ψ to property mass. So, if you now write that this ψ is this ρ we say that this was equal to ρdV . So, we can write m we can basically change the representation of ψ to mass, we can say m is equal to essentially ρdV and then we can write the Reynolds transport theorem for this whole thing.

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Conservation of Total Mass

Following RTT, the rate of change of mass is equal to sum of change of mass in C.V. and flow of mass across the control surface

$$\frac{\delta m}{\delta t} = \int_V \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} \right) dV = 0$$

Total mass is conserved in chemical reactions:

$$\frac{\delta m}{\delta t} = 0$$

Therefore: $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$. (Continuity equation)

$\frac{\delta m}{\delta t} = \int_V \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} \right) dV$ $\Psi = m$ $\Psi = \int_V \rho dV$
 $\Rightarrow \Psi = \rho$

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And that will see if as noting but so instead of capital psi we have replace with m replace capital psi with m. And we see that this is nothing but integral of volume d partial d rho partial d t plus divergence of rho v or integral over d V. So, now we know that total mass is conserved when there is chemical reaction. So, of course, this d m d t there cannot be no rate of change of mass possible and this then this thing is possible this thing is equal to 0, and then this becomes is equal to 0 so that is what you get. So, if the integral and this b because this d V is the essential arbitrary, so we can remove the integral, we can remove this d V and remove this integral sign. So, what will get is nothing, but this inside this d partial d rho partial d t plus divergence of rho v is equal to 0.

So, just to recap what we did because this is so important that is how we can understand the other things. I will just repeat again. So, we just apply the Reynolds transport theorem d psi d t is equal to is equal to integral v dou psi d t plus divergence of psi v vector times d V. And now if we write that psi is equal to m, and then it means that this implies that psi is small psi is nothing but rho because capital psi is equal to integral was equal to integral psi d V.

So by obviously, v then small psi is equal to rho and then we can say that dou m dou. If in the sense is arbitrary we can remove the integral side and we can convert this integral equation to this partial differential equation which is nothing but d partial d rho partial d t

plus divergence of rho v vector and that must be equal to 0. Because there is no rate of change of no mass change is possible. So, this is our continuity equation.

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Conservation of Total Mass

Following RTT, the rate of change of mass is equal to sum of change of mass in C.V. and flow of mass across the control surface

$$\frac{\delta m}{\delta t} = \int_V \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} \right) dV = 0$$

Total mass is conserved in chemical reactions:
 $\frac{\delta m}{\delta t} = 0$

Therefore: $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$. (Continuity equation)

RTT is similarly applied to derive species transport equation, momentum conservation, and energy conservation equation

Similarly, we can we can apply the Reynolds transport theorem to device to derive the species transport equation, momentum equation and energy conservation equation. So, this all this will just derive right now.

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Species Transport Equation

$$\frac{\delta m_i}{\delta t} = \int_V \left(\frac{\partial \rho_i}{\partial t} + \nabla \cdot \rho_i \mathbf{v} \right) dV = - \int_S (\rho_i \mathbf{V}_i \cdot \hat{\mathbf{n}}) dS + \int_V w_i dV$$

Sources and sinks of $\frac{\delta m_i}{\delta t}$:

- Volumetric (from reaction, w_i): $\int_V w_i dV$
- Surface (from diffusion flux, \mathbf{V}_i): $-\int_S (\rho_i \mathbf{V}_i \cdot \hat{\mathbf{n}}) dS$
 $\mathbf{V}_i \cdot \hat{\mathbf{n}} > 0 \Rightarrow$ loss, hence negative sign

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot [\rho_i (\mathbf{v} + \mathbf{V}_i)] = w_i, \quad i = 1, 2, \dots, N.$$

Similarly just we derive write m i v just we wrote that psi i is equal to m i we can write psi is capital psi is equal to m i and then it means that the small psi is nothing but rho i

that is a partial density of the species i . And then we can write $\frac{d m_i}{d t}$ is equal to $\int dV \int \frac{\partial \rho_i}{\partial t} + \text{divergence of } \rho_i \mathbf{v}$. Now, please note that this is the bulk velocity, but now interestingly this is not for the total mass. So, of course, the total mass is conserved, but in this case, there can be sources and sinks of $\frac{d m_i}{d t}$ that is a mass of a particular species need not the rate of change of the mass of a particular species inside a combustion involvement. Of course, will may not be zero suppose this m_i is i represented by the by methane a fuel.

So, of course, before and after combustion or in a as the flow is happening if we suppose there is a flow, and there is a flame, this is a flame you have. And suppose m_i or ρ_i will be large here if say i is equal to mass of CH_4 will be very larger, but that will be equal to 0, there will be no mass of CH_4 here right. So, of course, there will be we need to find out some sources and sinks. And those sources and sinks basically one is a volumetric which comes from reaction that is this is given by this $\rho_i \frac{d V}{d t}$, this d is given by this $w_i \frac{d V}{d t}$; w_i is nothing but the reaction rate and that we have learnt, but it is different units, we will come to that. It is actually units of mass. So, this is different this is slightly just very slightly different from the reaction rate that we have seen.

Whereas, this surface we will also see that there can be also surface fluxes especially from the diffusion flux v_i and that can be given by the diffusion velocity capital V_i . And that will be given by this integral about the surface with the minus sign and given by $\rho_i \mathbf{V}_i \cdot \mathbf{n} dS$, \mathbf{V}_i vector is the species diffusion velocity. And now this since this $\mathbf{V}_i \cdot \mathbf{n}$ is essentially zero which are which represents loss and hence we have the negative sign because that contributes to make it as a source term and that to represent the flux is coming inside from outside.

So, as a result this will be we can write is that. So, this is the equation, but this is not equal to 0, but instead it is this equation is nothing but minus integral of $\rho_i \mathbf{v}_i \cdot \mathbf{n} dS$ plus integral $w_i \frac{d V}{d t}$. Of course, you can now convert this dS this control integral over the surface to a control volume and this is now then it is now balanced. So, what I want to say is that the rate of change of m_i inside the system which is residence inside this control volume. So, as a result this rate of change of this m_i at the control volume is given by this two things. That is number one there can be a species flux which is the flux of species carried by this molecular diffusion velocity and also it

can change due to the reaction rate that is happening inside which is volumetric in nature happening inside the control volume.

So, these two contributors will now balance the rate of change of the mass of the species i inside the control volume. And when you apply the Gauss divergence theorem to this and convert this to a volume integral, you can basically transport it into this direction into the left hand side. And as a result, you can write this simplified equation which is $\partial \rho_i / \partial t + \text{divergence of } \rho_i \text{ times this is the bulk velocity}$. And this is the diffusion velocity.

So, and this is essentially is equal to the and this is of course, after you are remove the integral and just gone into the partial for differential equation form and this is given by the reaction rate w_i and which is this is of course, in a mass form. So, this w_i also in a mass form, units a mass essentially not in some mass, but in some mass per grams per cubic meter second that is the typical unit of this one. And this is coming of course, true for any species.

So, thus what we sees that essentially this is our species balance equation. It looks simplified, but actually it is not because we have not specified anything about this species diffusion velocity. And we will need this some constitutive relations for this $\rho_i V_i$ to be supplemented to close this equation because we have not specified anything about this. Now, of course, we leaves our knowledge of chemical kinetics that we have studied in sufficient details to use this two model to basically to describe this term which is the basically the rate at which the species i changes because of the chemical reactions. So, this is the source term in this species equation.

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Conservation of Momentum

$$\Psi = M, \psi = \rho \mathbf{v}$$

$$\frac{\delta \mathbf{M}}{\delta t} = \int_V \left(\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \rho \mathbf{v} \mathbf{v} \right) dV.$$

Sources and sinks of $\frac{\delta \mathbf{M}}{\delta t}$:

- **Surface source** (by stress, \mathbf{P}): $\int_S (\mathbf{P} \cdot \mathbf{n}) dS$
 $\mathbf{P} \cdot \mathbf{n} > 0 \Rightarrow$ system exerting force on surrounding, hence negative sign
- **Volumetric source** (by body force, \mathbf{f}_i): $\sum_{i=1}^N \int_V \rho \mathbf{f}_i dV$

$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot \rho \mathbf{v} \mathbf{v}$	$= -\nabla \cdot \mathbf{P} + \rho \sum_{i=1}^N \mathbf{f}_i$
$\rho \frac{D\mathbf{v}}{Dt}$	$= -\nabla \cdot \mathbf{P} + \rho \sum_{i=1}^N \mathbf{f}_i$

Now, we can also use the conservation of momentum. Now, psi is equal to psi is equal to the momentum which is m times velocity. So, this is essentially m times v and now then becomes in the partial the small psi this was the extensive property, this is the intensive property. This is the essential as specific property then small psi essentially becomes equal to rho times velocity. And then the rate of change of momentum inside this is essentially integral of we just replace this thing into the which is replace the small psi in this, and we get that essentially partial d rho d rho v d t plus divergence of rho v vector v vector over this.

Now, of course there can be forces acting on this control volume. And there can be surface forces in terms of flux stress and pressure. And this capital P is essentially full surface force tensor and it will contain also force from pressure two different viscous stress etcetera. And there can be also we have volumetric source like a body force f i though this will not be of our interest mainly in this course, which comes from this f i, but will keep this one for generality. This will be of course, very important because as will see later all this will contain both a pressure component as well as the viscous components. And this viscosity will actually come into this. So, this is the form that I want to remove the convert this volume this integral form to a partial differential equation form.

What we get is nothing but this partial d rho d t which is the transient term then we get this advective term both are actually in the both are nothing but this in this is nothing but the auxiliation of the fluid and this auxiliation is caused by this surface by the gradient of the of this pressure tensor which is nothing but the force. And this force can also be exhorted by a volumetric source and from body force. And this is in another form this way we have get the total D v D t which is the total acceleration is given the minus gradient of p pressure tensor which is nothing but the total force and plus the body force. And we will later break this up into the actual pressure and viscous forces and will eventually neglect this.

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Conservation of Energy

$\Psi = E, \psi = \rho e + \rho v^2 / 2$ ↑ internal energy ↑ kinetic energy

$\frac{\delta E}{\delta t} = \left[\frac{\partial \rho(e + v^2 / 2)}{\partial t} + \nabla \cdot \rho \mathbf{v}(e + v^2 / 2) \right] dV$ → LHS

Sources and sinks of $\frac{\delta E}{\delta t}$:

- surface source (by energy flux \mathbf{q}): $Q = -\int_S (\mathbf{q} \cdot \mathbf{n}) dS = -\int_V \nabla \cdot \mathbf{q} dV$
- surface source (by surface stress): $W_s = \int_S \mathbf{v} \cdot d\mathbf{F}_s = -\int_S \mathbf{v} \cdot (\mathbf{P} \cdot \mathbf{n}) dS = -\int_V \nabla \cdot (\mathbf{v} \cdot \mathbf{P}) dV$ +
- volumetric source (by body force, \mathbf{f}_i): $W_v = \sum_{i=1}^N \int_V \mathbf{v}_i \cdot d\mathbf{F}_{r,i} = \sum_{i=1}^N \int_V \mathbf{v}_i \cdot (\rho_i \mathbf{f}_i) dV = \sum_{i=1}^N \int_V (\mathbf{v}_i + \mathbf{V}_i) \cdot (\rho_i \mathbf{f}_i) dV$ X

$\frac{\partial \rho(e + v^2 / 2)}{\partial t} + \nabla \cdot \rho \mathbf{v}(e + v^2 / 2) = \rho \frac{D(e + v^2 / 2)}{Dt} = -\nabla \cdot \mathbf{q} - \nabla \cdot (\mathbf{v} \cdot \mathbf{P}) + \sum_{i=1}^N (\mathbf{v}_i + \mathbf{V}_i) \cdot (\rho_i \mathbf{f}_i)$ X

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Finally, the conservation of energy: now this is the most actually this is the most complex situation and this is also the most important when it comes to combustion because in combustion temperature is the king and essentially we will see later that from this energy, we will derive useful form for temperature. So, this transport of temperature or this transport of thermal energy, we will be coming from this conservation equation. So, for now we start with the very modestly we write this extensive property that is capital psi is the total energy which is the total internal energy.

And then the corresponding a specific property small psi becomes density times the specific integral energy plus this is the kinetic energy component rho v square by e. So, this is the internal energy and this is the kinetic energy component.

So, once again proceeding similarly we can actually by the Reynolds transport theorem, the rate of change of this total internal energy inside the system which is resident inside the control volume is equal to the rate of change of this internal energy inside the control volume. And that happens due to the rate of change of that property inside the control volume plus the fluxes of this property that is coming through the control surfaces. So, this is the control rate of change of the property inside the control volume, this is the flux of that of the internal energy plus the kinetic energy that is coming from the surface integral convert into volume integrals using the Gauss divergence theorem.

So, this is the left hand side, this is the other rate of change, that is we also need sources and sinks because they are definitely be sources and sinks, because there can be a energy flux Q vector there can be heat flux vector. And that will actually in the volumetric form appear though it is actually in the surface form in this form Q vector dot it is the you consider this as essentially heat flux vector; heat flux vector dot normal vector in the surface integral which becomes essentially equal to the divergence of heat flux vector volume integral. And then there also be surface stresses, which is if you remember flow work and that is the work done by pushing work done by pushing the fluid because of the by the external surface forces like pressure. So, to account for that need to the will come into this and this is that form

And also there can be volumetric sources of body forces which can be also coming which can do some work and by body force and this is also coming. This typically once again will not be will not be importance in this thing and will not consider this much, but all these things, these things very, very important I will inform it in integral form integral part of our integral meaning very important part of our and analysis here.

So, if you write thing down this is the total thing, this is the essentially the though it is RHS is here we had actually when you write down the governing equation this forms LSH and this plus this forms the RHS - right hand side, this from left hand side, this from right hand side. Say, if you collect this and if you collect this, what you get is this is your transient term $d\rho$ times internal energy specific integral energy plus kinetic energy by γ viscous by 2 partial d t partial d t plus this advective term, this divergence of ρ velocity vector times specific internal energy plus v square by 2. This is can be totally written in a this total material derivative format that is ρ times total derivatives of e plus v square by 2 divided by d t

Then that is equal to the sources and sinks. This is the surface flux of heat that can come and that is given by divergence of q vector. Heat flux vector and then there can be this flow work which is basically the work done by the external surface forces by pushing the fluid in. And then there can be this force due to the then this can be the work by the body forces as we said this will not be of important we will not consider this. Because will not really consider body forces will not even consider gravity in this mostly in this thing. So, though gravity can be important because of the buoyancy effects, but especially when we talk about fires, but in terms of this combustion course will not consider also much gravity and acceleration due to gravity will not consider and will not consider any body forces as such.

Though there can be important in certain circumstances like electromagnetic ionic wings etcetera, if you took plasma assisted combustion this sort of forces might become important. But for this for this course will not consider this will our equation will essentially we restricted to this part only.

So, now, if we summarize, so using starting from a very generalized Reynolds transport theorem for any property capital ψ and we started with notion that capital ψ is essentially an extensive property of a system. And with the system is essentially coincident inside a control volume and then we can write our loss for that system and then we can write a loss for the control volume. And this Reynolds transport theorem that equates this to loss by considering the by the additionally we considering in addition to considering what happens in the rate of change of the control volume. We additionally consider what comes in and what goes out of the control volume the flux of those properties.

And then this flux of this property is actually come in surface form and then we converted this surface actually a surface integrals and we converted this surface integrals into the volume integrals using Gauss divergence theorem. And then we apply this for a generalized volume, and we apply this for mass, we apply this was species we apply to this momentum. For mass there is no balance extra source sink required, because the mass is essentially equal to the rate of change of mass inside the system coincident with the control volume and the rate of change of mass in the control volume plus the mass flux coming in the mass flux is going out that is equal to 0.

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Summary of Conservation Equations

Continuity: $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$

Species: $\rho \frac{DY_i}{Dt} = \rho w_i + \nabla \cdot (\rho \mathbf{V}_i)$, $i = 1, \dots, N$

Momentum: $\rho \frac{D\mathbf{v}}{Dt} = -\nabla \cdot \mathbf{P} + \rho \sum_{i=1}^N \mathbf{f}_i$

Energy: $\rho \frac{De}{Dt} = -\nabla \cdot \mathbf{q} - \mathbf{P} : (\nabla \mathbf{v}) + \rho \sum_{i=1}^N Y_i \mathbf{f}_i$

The conservation equations are supplemented (completed) by the specifications of

- Diffusion velocity, \mathbf{V}_i
- Pressure tensor, \mathbf{P}
- Heat flux vector, \mathbf{q}
- Reaction rate, w_i

So, we do not need additional source in terms, but when it comes to like things like species when it comes to things like species we need additional sources and sinks. There can be sources of sinks in terms of this reaction which can generate a depletion, a particular species and also there can be species flux coming in crossing the control over surface and we need to account for that. Momentum also the rate of change of momentum is given by this $\rho \frac{D\mathbf{v}}{Dt}$ then that can be changed by surface forces through pressure or rather the gradient of pressure and also by body forces. Once again this is not important will not consider this will not consider this.

And also in terms of energy will see that the rate total internal specific internal energy that will be changed here we actually can do some take the dot product of this momentum equation. And subtract with this equation and we can arrive at a energy equation for purely for specific internal energy and that is what we have done here. And will see that we are derive this from divergence of this c flux times p tends are constructed twice with divergence of \mathbf{v} , and then we can neglect this body force term. So, this is what we have done.

Now, we have these complete conservation equations ready. We have conservation equations for continuity conservation of equations of species, we have conservation equation of species, we have conservation of species of momentum, we have conservation of equation of species, we have conservation of equation momentum, and

we have conservation of energy that is all the conservations we need. But then these equations are not complete and this forms we are not be able to do solve them. Why, because we see that there are very interesting things which we do not know, we do not know about how this V_i will look like we have equations for v we have equations for the bulk velocity, but we do not have any equation for V_i which is the species diffusion velocity.

Similarly, we do not have any constitute of relation for pressure, we need to supply that we what can be that can be this. So, this something that this V_i can be supplied this by fix diffusion law, this pressure this can be come from this equation of state. And this heat flux vector this divergence of q that can happen many things like can have heat conduction, Fourier law of heat conduction, it can have like radiations source and it can have also heat flux due to heat different heat contents of different species will see that all.

And also very, very importantly what we need is that we need to close this we need constant tribulation for this ω_i this w_i , but of course, we know w_i we can use this law of mass action that we have fully learned in the previous classes. And also we can use this that k that comes in front of this products of species raised to the (Refer Time: 39:36) exponents and then we can use them to basically come at reaction rate for w_i .

So, we will come at this will come to this, so this conservation equations are two supplemented by specification of the diffusion of velocity capital V_i , the pressure tensor capital p and the heat flux vector q and of course, a reaction rate w_i . And we will supplement this things we will come at this specific closures this auxiliary equations or this constitutive relations for this quantities in next class.

Thank you very much.