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Lecture – 07 Macroscopic Balances – I

Welcome today, we shall be looking into the Macroscopic Balances and this is macroscopic balance relates to all the things like mass for energy for momentum. So, this particular topic will be spread over a few lectures. So, this is the first lecture on the macroscopic balances.

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So, in this we shall be covering the conservation law in the integral form and then in the differential form.

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Conset • Consider a volu function of pos	vation in in Ime specific property Ition factor (r) and t	n tegral form (mass, energy or momentum) ime (t)	$\hat{\Phi}$ which is a
	Conserved property	φ.	
	Mass	Density or concentration	
	Momentum	Density x velocity	
	Energy	Density x specific heat x temperature	
	ayam (*)	

First let us see that, what is the conservation in integral form. So, for that we have to first consider a volume specific property for mass, energy or momentum and that is represented by say phi hat, which is a function of position vector r and time that is a whenever any kind of property is there that will change spatially as well as temporally means with different locations and with different times.

So, in general any property will be a function of both position and time and that position is given by the position vector r and time is given by t. Now please understand, this position vector r can be represented in various manner in various coordinate systems. So, whatever notations we are using now, this is independent of the coordinated system.

Now again it is understand that what we mean by volume specific property for mass, for energy and for momentum, here we is write in this table the conserved property and the corresponding value of the phi hat. Now, here you see the for mass it is the density or concentration, density when we are talking of the whole mixture then we talk of density and concentration when we talk of species by species ok.

So, it can be the density or concentration then for momentum it will be density into the velocity then for energy it will be density into specific heat into the temperature, that is the energy content or the momentum of a given mass. And, understand this density is the one, which is telling us mass per unit volume that is how each of these are becoming volume specific properties.

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Next we come to a particular equation and this is a very famous equation given by Reynolds and we call it Reynolds transport theorem and what is this is like this that this is the mathematical representation of this particular equation, here what it gives. Here first to understand this it let us first look at the control volume V and this left hand side tells us that how a particular a specific property is changing within a volume with time. So here, this integral is over the volume, that means, because it is volume specific so when I integrate over the volume, I get the total value ok.

So, this total value within a control volume and how is it changing with time. So, and this change what is happening, due to some influx or out flux from the control volume or in the control volume and due to some kind of generation. So, in effect this is the this particular term is showing the net influx minus influx and out flux and this is the generation and due to this influx out flux and the generation, what is happening inside the control volume and now you see that this particular flux is happening at the surface.

So, we are taking the surface integral and this F is representing the control surface and J representing the flow into or out of the control volume crossing the control surface. This is important the particular flow has to cross the control surface and this n F is the outward unit normal vector from the control surface and when we take the dot product because, this is a vector, these are vector when we take the dot product of the 2 vectors,

we get the flux and this last one is this the source term to account for any generation or consumption of this particular property within the control volume ok.

Like for example, in case of mass balance or mass conservation, this q will represent some kind of reaction that might be either consuming the particular species or might be generating the particular species ok. So the now, you look at this that in this particular integral form that we are integrating over the whole control volume. So, over the whole control volume, this is the whole surface and this cyclic integral means, the surface is bounded ok. So, there is no gap between the surface. So, that is the meaning of the cyclic integral and this particular thing again, it is over the volume because, this generation is per unit volume.

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Now, you see pictorially we can also see that in we are drawing this particular control volume and here we are showing something is coming in and something is going out and this F is showing the control surface.

So now, you can see that this is the outgoing normal and depending on the theta value that theta means, the angle between the normal and the flow stream. Now here you see, the theta for the outgoing stream is acute that is less than 90 degree. However, for the input stream it becomes obtuse that is more than 90 degree and when you take the dot product that is cos theta ok.

So, this into this into cos theta you see that this gives us a positive value, whereas this gives us a negative value. So, automatically you see that by defining the dot product between the flux and the normal, we are able to account for the influx and out flux ok. So, it is very important that for you to know, how to draw this particular normal and normal is always outgoing, never make it in going ok.

Now, this particular system again we take on a actual the system. Now here, we have been considered a flow through, a flow divider, what it means? That a particular flow is coming and then it is getting divided into 2 streams. So here, we find that we have 1 input and we have 2 outputs and again for the input side, what we do? Again, we draw this particular normal that is outward normal from this surface and this is the incoming stream. So, we can take the dot product between the 2 and which we shall get a negative value whereas, for the outgoing streams we find the dot product between this flux and this particular normal will lead to positive values ok.

So, this is how we can see that we are able to implement this particular flux concept. One thing is this that in this particular control volume, we have neglected any kind of reaction; that means, any kind of mass generation or consumption. So here, we are just showing that how the mass is getting conserved by this particular example, similar things can be done for the energy and for the momentum transfers also.

Conservation in differential form • When control volume ${\cal V}$ becomes infinitesimally small, we get differential form by applying Gauss divergence theorem to the surface integral to convert it to a volume integral. · Differential form is given by $\partial \Phi$ $\overline{\partial t} = -\nabla J + \hat{q}$ Cartesian coordinate: $\frac{\partial J_x}{\partial x}$ + дy $\frac{1}{r}\frac{\partial rJ_r}{\partial r} + \frac{1}{r}\frac{\partial J_{\theta}}{\partial \theta} + \frac{\partial J_z}{\partial z}$ Cylindrical coordinate: $\frac{1}{\partial r^2 J_r} +$ $\frac{\partial(\sin\theta J_{\theta})}{\partial(\sin\theta J_{\theta})} +$ 1 1 ðJφ Spherical coordinate: -2 дө dr $r \sin \theta$ r sin 0 da SWay 4 1 / / /

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Now, let us go to the conservation equation in differential form. Now way means a differential, what it means is this we choose a very small control volume that is, we call it infinitesimally small. Now, this small is arbitrary again and this is a relative concept, how small? It will depend on the overall system and in that overall system the, what kind of how closely one wants to analyze that will define the size of the control volume. Anyway, we say that we are choosing a very small control volume and then when we write these conservation equations, we get differential form and here we apply the Gauss divergence theorem to the surface integral to convert it to a volume integral.

So, I will not be going into the details of this Gauss divergence theorem, which is covered in some mathematics course. So, without going into detail we simply right the Gauss divergence theorem and put it in this fashion. Now what we find here? That the same integral form of the conservation equation has been has been reduced to this particular form using the Gauss divergence theorem and we find that this divergence means here, we get the divergence of the vector J and this divergence is the dot product of the nabla and the particular vector.

Now, what is nabla? Nabla again is defined differently in different coordinate system, it basically gives us the 3 dimensional change of a given vector ok. So here, we have written for Cartesian coordinate, this will this nabla dot J will look like this. For the cylindrical coordinate, it will look like this and for the spherical coordinate it will look like this. So, depending on the coordinate system, this delta dot J will change it is form and in my previous lecture, I have also given you the relationships between the various coordinates in the systems.

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Now, in this particular conservation law what we encountered, we encountered this flow or transport terms. So, let us see what it means. Now total flow can be divided into 2 components, one component is the convective flow, another is the diffusive flow. Now, the convective flow is given by J C and diffusing by J D. Now this convective flow means, which is happening due to the motion of the particular fluid or the particular material and the motion is given by some velocity field v. So, this J C is given by the particular property and by and the particular velocity field.

So, when we take these 2 product, we get the convective flow ok. Now in this a particular equation, we obtain the value of the velocity field by solving the momentum balance equation. So, you can see that if we are looking at the mass balance momentum balance atomically creeps in and they become coupled. On the other hand, when we talk of the diffusive flow, it depends on the gradient of the potential some potential. Now in simple terms, it means that the diffusive flow will be happening whenever there is some kind of gradient for example, if you look at heat transfer, it will occur only when there is a temperature gradient; that means, the temperature will representing this value ok.

And similarly, whenever there is a mass transfer like for example, you are trying to dissolve sugar in water or milk. Now what happens, because there is initially there is a the there is a gradient of concentration. So, you find that sugar is going inside the liquid ok.

So, in that case the concentration will be this value ok. So, that is what that it means that diffusive flow occurred due to gradient of the potential and this is given by this particular thing that might negative of D into this again this nabla and into this scalar understand, this has scalar field, now this scalar field is now being converted to a vector field ok.

Now this D in general is a diffusive coefficient, it can be mass diffusivity, it could be a momentum diffusivity, it could be thermal diffusivity ok, depending on which kind of conservation property we are applying. So here, we are putting D as an arbitrary parameter ok. And as I mentioned that this sign represents some mass balance it will differ for mass balance for momentum balance and for energy balance.

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Next we come to source term. Now, what is the source term? This will be something which is other than the diffusive term or the convective term, anything other than that will be the source term. Now why this source term comes? It can come due to various factors, one factor is the chemical reactions.

Now, I have shown you some chemical reactions, which are very which are important for us. For example, here you see that how the methane is getting combusted to generate some energy in that it is giving us carbon dioxide and water and this methane is get we are getting it from the cng that is the compressed natural gas or lng that is the liquefied natural gas. So, this is a very common thing which we are using to get energy that is this methane is and a fuel ok. And this another, example that how the water can be disintegrated by electrolysis to give us hydrogen and oxygen. So here, this is another kind of reaction.

So, this can be this kind of simple reaction in terms of the molecules involved, not in terms of the conditions of course, another kind then we can require quite complex reaction can be there that in this we see that there is some complex molecules and to get a another product from this molecule, we have to follow several steps with several temperature conditions and several kinds of reagents to obtain the final product. So, reactions can be of various types, but they all lead to some kind of source term.

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Another source term can be due to energy dissipation or conversion and this can be the due to heating due to noise or friction and it could be from compression or density changes within the system. Now here, I have shown an example that how energy can get dissipated? Whenever we are writing a say a car, we are burning some fuel like a diesel or petrol. Now what happens that whatever after combustion of this diesel or petrol, whatever the energy is coming out all the energy is not used up to drive the car.

We find that there will be some heating up in the system and will be quite noises. So, all these are the sources of energy dissipation in the system and you will find that out of the whole energy of combustion generated only a part will be used up further this kinetic that is a useful energy ok. So, but this is also if these all these energies will be part of the source terms.

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Next we come to some other source terms due to the pressure field for example, turbine in a turbine you know that we put some kind of pressurized gas and the turbine propeller rotates and that is how we are able to convert that pressure energy into some useful energy. Then we have a gravitational field then gravitational field we have the aircraft, space vehicles, which have to be designed. So, that they can overcome the gravity and move and then we have electrical field and magnetic field, we generally come together, we call them electromagnetic forces and here I have shown you some day to day devices which depend on the electromagnetic forces and you find that this is this thing come because, there is some kind of a magnet in the system and there can be a some coil, which if you if you are passing some electric through the coil it will be generating some magnetic field or vice versa.

So, these are some devices we have found see and you see also for example, whenever we are running a motor you find that on running for a long time the motor gets heated up, this heating is nothing, but the dissipation of energy ok. So, all these things are the source terms. Now, this source term depend on the potential again corresponding to equivalent extensive property characterizing the process system. For example, we have concentration, temperature etcetera, they are the as I told you earlier, these this will be depending on that what kind of dissipation we are having whether, we have mass dissipation we have, whether we have anti dissipation depending on that it will be this value will be having different connotations.

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General operator form of differential			
conservation equation			
Incorporating the transport terms in the differential conservation equation			
we get $\partial \widehat{\Phi}$			
$\frac{\partial t}{\partial t} = -\nabla (f_c + f_p) + \hat{q}$			
$\frac{\partial \Phi}{\partial t} = \nabla (D\nabla \varphi(r, t)) - \nabla (\widehat{\Phi}(r, t) v(r, t)) + \widehat{q}$			
This is coordinate-system independent differential conservation equation			
• Generally nonlinear due to form of \widehat{q} and/or when D is not constant			
• Conservation equations are generally coupled due to \hat{q} when both mass and energy conservation equations are written:			
✓ Reaction term is function of both concentration (mass intensive property)			
and temperature (energy intensive property)			
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Now, after learning about this integral difference operator, now what we do? We go to the differential form of the conservation equation in a operated way operator means, now we shall be we introduced the nabla operator to you. Now, what we shall see? That we are just in putting the values of J here and we are rewrite in the same equation as I wrote earlier. So here, I am writing that minus nabla of J C plus J D for J and now we are taking them out. So, first we find that this J D we are putting as minus D, this nabla into psi rt and this negative gets cancel, it will become positive and this becomes this JC, we are putting this value. So, it is retaining the negative value and plus this.

Now in this particular equation is coordinate independent, it does not depend which coordinate that is they say general statement without any dependency on the coordinate and this equation now can be modified as per the case. For example, if the deficit it is constant it is not changing then we can take it out of this particular, the nabla operator and then this becomes delta square then sorry nabla square this psi rt.

The nabla square means. So, in say example in the rectangular coordinate, this nabla square will be del square by del x square plus del square by del y square plus del square by del z square. So, this kind of simplification can be done from case by case basis and

sometimes if you find that the diffusive a contribution is less than the convective contribution then we can drop this particular term. And vice versa, if you find for some system, the convective term is less dominant than diffusive term then we can also neglect this and in some systems we can also drop this term out if there is no generation or consumption.

Now, this system is general non-linear because this q and D are not constant and many times we find that these equations are coupled; that means, as I showed you earlier the momentum equation and the mass balance may be coupled, the mass balance will be coupled with the energy balance equation. Because, if in the mass balance we have the densities and the densities are functions of the temperature and temperature can be obtained from the energy balance equation and the energy balance equation also we are having the density specific etcetera.

So in that we find that everything becomes a coupled set of equations. So, we can get in general non-linear coupled differential equations. Now this reaction term is the one which many a times for the source term reaction term can give rise to this coupling and this reaction depends on the concentration, which can be obtained from the mass intensive property and this temperature that is the energy intensive property that is we are obtaining them either from the mark and from the mass balance and from the energy balance equations.

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Now, we come to another important concept that is the lumped parameter system, in this lumped parameter system it may be steady or unsteady and it is basically a scalar field of intensive properties that is a function of only time; that means, there is no dependence on the location. And, because there is no dependence of location, we find from the previous equation that the nabla operator will not be the will not be coming into picture.

So, only we have the left hand side in which we have the time derivative. So, it leads to a ordinary differential equation. Example is this, when we mixing of a sugar in milk to bring the whole system at a some same concentration that is it becomes an homogeneous mixture, what it means that there is no to the concentration gradient that is we can see that there will not be any variation of sweetness of the milk at different locations and then on the energy side if we are mixing a hot and cold liquid, what we find that ultimately they will bring to some uniform temperature that that is also is a means that we are avoiding any kind of locational variation of the particular property that is the temperature.

And in these cases, we apply the integral form of the conservation law and when we do. So, we find that the flux become equal to J C because, the diffusive term is gone because, there is no gradient. So, the total flux is purely depends on the convective flux.

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Now, coming to the control volumes because, whenever we are making such kind of balances we need to select a control volume. So, what is control volume? A control

volume represents some elementary region, which will be representative of the whole system and in this we see that the we can write the conservation law with the appropriate assumptions.

So, these control volumes are also known as balanced follows because, over the control volume we are applying some kind of balanced equation for the conservation. So, when there is some special variation of the conserved property then we have distributed parameter system. And, for this kind of system, there will be representative balance volumes are defined in which the conserved property is to be taken uniform; that means, we have a bigger control volume. But, when we find in a bigger control volume, we have distribution of property then we make smaller control volumes within the bigger control volume.

And in each of these smaller control volumes, the all the properties are taken to be uniform even though in the overall there will be distribution, but in the differential control volume, there will not be any distribution of the property. And different control volumes like for mass energy and momentum and these one energy balance may be having more than one mass balance; that means, it is not necessary that the number of control volumes for mass balance is same as that for the energy balance.

So, these number of control volumes may differ and I will show you by example that how we find that energy balance and mass balance control volumes, may not count the same and these control volume concept form the basis for the modeling any system.

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Now let us see typical types of control volume, one can be that if you are talk of fluids, it can be single or pseudo phase single means there will only vapor or liquid or solid or pseudo phase; that means, suppose we have some kind of emulsion, where we have 2 immiscible liquids then we for simplicity sake, what we can do? We can assume an overall phase and because, it pseudo phase which will be having some properties of some average properties of the 2 constituting phases.

Then we can have perfectly mixed phase like in case of gaseous mixture or we can have uniform or homogeneous flow pattern where there is no looking a locational gradient.

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Now, for solution of control volume this is very important, how we select? Now, selection is arbitrary, but depending on the selection we make our analysis may get simplified or may get complex. So, with experience it comes to us also that how to select a control volume before we start writing the balanced equations and only thing is this a control volume should ensure accounting for all the inflow and outflow of the conserved properties. That means, if there is a energy balance to be made we have to make sure that the control volume is made in such a manner that it cuts the surfaces in a way that we can take into account all the incoming energy and all the outgoing energy.

If this control volume does not do that then we will not be able to make the proper balances. So, it is that is what it says that a control volume must ensure that it can take into account all the inflows and outflows, may be fixed or moving, may be rigid or flexible and here in this particular figure, I have shown you the meaning of this. Now, you see there is they there is a from the nozzle some fluid is coming out and this nozzle is not moving. So, we call it a fixed control volume similarly, here we have a helicopter. Now, when the this helicopter fan is moving, we find that the air is getting also rotated and in this case we find that this is because of this propulsion, this helicopter is moving forward ok.

So, if we take this as the control volume, we find that this is the helicopter is moving. So, we call it a moving control volume, on the other hand if I look at a balloon. Now what

will happening that whenever you are inflating or deflating a balloon for example, you can also do the same thing with a football or a tube of the cycle. So, in whenever you are putting some kind of air, you find it inflates; that means the volume is changing.

So, we call this a deforming control volume whereas, in case of say pump, when through a pump some fluid is flowing, but the pump structure is not changing it is remaining same. So, it is a rigid control volume. So, depending on the different types of the processes, we may have these variations and we can have combinations like we can have fixed and rigid control volume, we can have fixed a flexible control volume, we can have moving rigid control volume and moving flexible control volume. So, all these kind of combinations are possible, whenever you are selecting the control volumes.

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And here as I was telling you is an example of an evaporator, where we find that that energy balance and mass balance control volumes may be different. So, in the first figure what we see that we are taking the control volume as the overall evaporator and this evaporator a some feed is coming. And, this is feed is liquid generally and this is being heated up with some steam and due to which, the liquid is converting to vapor, we are taking the vapor out from the top, liquid from the bottom.

And here, we can make a mass balance, energy balance on over the whole evaporator, if you do that we will be obtaining that how the total mass inside the evaporator is changing or how much energy is getting accumulated in the evaporator. On the other hand, if we want to know that how the liquid level is changing due to evaporation that cannot be known, if we choose this particular control volume in that case we have to choose 2 control volumes, one will be for the vapor phase, another will be for the liquid phase.

Now, in this way we shall be able to determine the change in the liquid level due to the evaporation ok, but at the same time if you want to still know the energy in the system in and how much energy is accumulated then we need not choose these 2 volumes separately because, the total energy is the summation of the energies of the 2 phases.

So, for the energy balance we can still go with the previous control volume that is the total evaporator. So, you can see that in this case, the energy balance control volume is having the 2 mass volumes within it. So, in that way we is conclude that it is not necessary that the number of control volumes for the mass and the energy must be the same.

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Now, whenever see mass lumped parameter, we mean that there will be homogeneity of the states within that control volume for global description of the system and the scalar field is lumped into some representative value; that means, we are attributing only one value of the intensive variable whether, temperature pressure concentration etcetera, within the control volume and this lumping is coming only when there is a where system is well mixed and this that is why they are called well mixed system. This mixing brings the whole system at a given state and this is applied for various cases like process design, process safety then if I want to start up or shut down a particular process and for process control and diagnostics for all these systems, we do not need to know the spatial variation of the properties their overall behavior that is inlet and outlet behavior is good enough. So, we go for the lumped parameter systems.

Thank you.