Heat Transfer And Combustion in Multiphase Systems

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Lecture 08
Interfacial heat and mass transfer-II - Interfacial dynamics, Instabilities of the interface

So, in the last class, what we did was, in the last lecture that we try to work out the integral formulations of the mass and the momentum equation okay. So, the point that we stopped was that we defined that how the continuity equation or the mass conservation equation can be written. And we also propose the momentum equation in its integral version.

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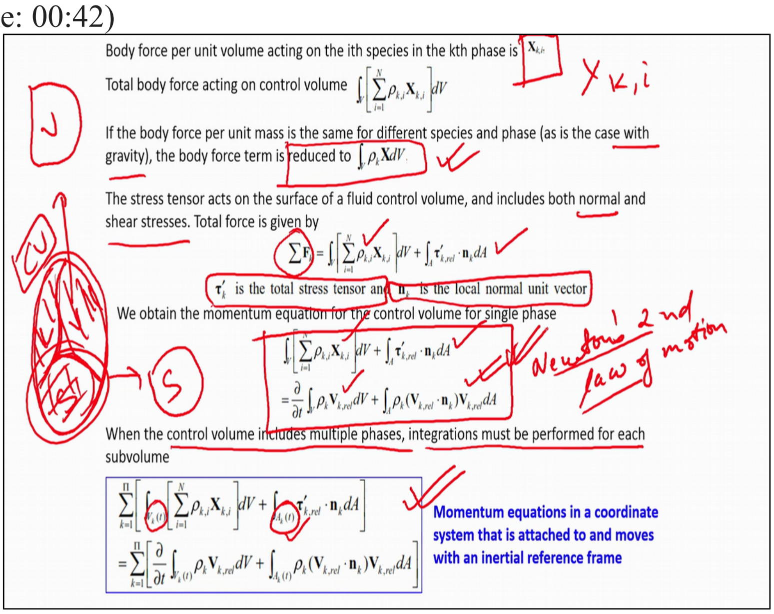

Body force per unit volume acting on the ith species in the kth phase is $\mathbf{X}_{k,i}$

Total body force acting on control volume $\int_V \left[\sum_{i=1}^{N} \rho_{k,i}\mathbf{X}_{k,i}\right] dV$

If the body force per unit mass is the same for different species and phase (as is the case with gravity), the body force term is reduced to $\int_V \rho_k \mathbf{X} dV$.

The stress tensor acts on the surface of a fluid control volume, and includes both normal and shear stresses. Total force is given by

$$\sum \mathbf{F} = \int_V \left[\sum_{i=1}^{N} \rho_{k,i}\mathbf{X}_{k,i}\right] dV + \int_A \boldsymbol{\tau}'_{k,rel} \cdot \mathbf{n}_k dA$$

$\boldsymbol{\tau}'_k$ is the total stress tensor and $\mathbf{n}_k$ is the local normal unit vector

We obtain the momentum equation for the control volume for single phase

$$\int_V \left[\sum_{i=1}^{N} \rho_{k,i}\mathbf{X}_{k,i}\right] dV + \int_A \boldsymbol{\tau}'_{k,rel} \cdot \mathbf{n}_k dA = \frac{\partial}{\partial t}\int_V \rho_k \mathbf{V}_{k,rel} dV + \int_A \rho_k (\mathbf{V}_{k,rel} \cdot \mathbf{n}_k)\mathbf{V}_{k,rel} dA$$

When the control volume includes multiple phases, integrations must be performed for each subvolume

$$\sum_{k=1}^{\Pi}\left[\int_{V_k(t)} \left[\sum_{i=1}^{N} \rho_{k,i}\mathbf{X}_{k,i}\right] dV + \int_{A_k(t)} \boldsymbol{\tau}'_{k,rel} \cdot \mathbf{n}_k dA\right] = \sum_{k=1}^{\Pi}\left[\frac{\partial}{\partial t}\int_{V_k(t)} \rho_k \mathbf{V}_{k,rel} dV + \int_{A_k(t)} \rho_k (\mathbf{V}_{k,rel} \cdot \mathbf{n}_k)\mathbf{V}_{k,rel} dA\right]$$

Momentum equations in a coordinate system that is attached to and moves with an inertial reference frame

Now remember in those equations okay we define that there is a body force term okay which is strictly given by X ki this is a continuation of last lecture. Now the body force term in most of the cases it is gravity okay. So, if it is gravity the body force term is reduced to a form like this okay. So, the stress tensor, so, this is the body force term okay.

Now the other forces that are acting on the control volume on the fluid control volume okay includes both the normal as well as the shear stresses, right. So, shear stresses you know what shear stresses are, okay. So, from your undergraduate fluid mechanics knowledge, so it is the total force is basically nothing but the sum total of the body force and the total stress.

So, tau k this particular thing is nothing but the total stress tensor and nk is basically the local normal unit vector, okay. So, the total momentum equation therefore can be written in this particular form, okay. So, what can we say this particular term is a rate of change of momentum within the control volume, this is the momentum flux basically these two constitutes the convective derivative portion.

This is nothing but the body force term and this is the total stress term, okay. So, this is nothing but Newton's second law okay, law of motion, got it. Now if we, if the control volume includes multiple phases. If you recall that particular diagram where we had say three phases, okay. So, this is like your control volume, three phases. So, this is liquid this is vapour, this is solid these are basically the areas.

This can be actually 3d and this is the volume okay. Now if it contains multiple phases then you need to perform this integral form for each of those sub volume right. So, sub volume indeed this is one sub volume, this is another sub volume that is another sub column, right. So, if the phases are very well separated and things like that you can actually have these two as your sub volumes, okay, got it.

So, that is an interesting assumption over here that the control volume is occupied by several phases. In this case it is solid liquid and vapour, okay. So, when it is solid you have the solid part which is the solid part of the control volume. So, when you actually perform integration over multiple phases this is the final form of the equation that you get.

If you look at this form there are a couple of things the area Ak is basically the individual areas, the individual control surface for example if I look at this particular diagram once again you will find, if I take this out this is for example the area of the solid, okay. If I take that out, this particular area out, this is like the area of say the vapour right.

So, this is that area that we are talking about okay. Similarly these volumes are the individual sub volume the rest of the equation remains exactly the same, right. The rest of the equation is nothing but this, but it has been summed over all the phases, okay. So, that is the momentum equation that we did last class there we have reemphasized and said that what the momentum equation should look like.

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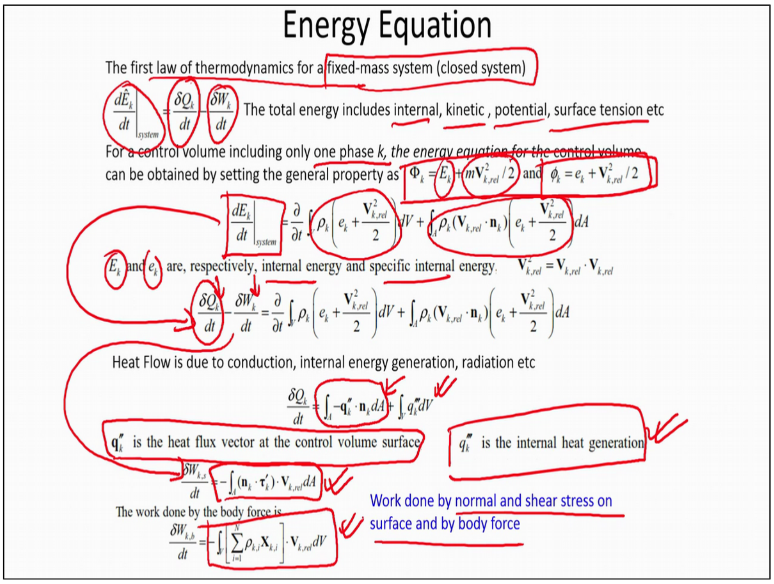

Energy Equation

The first law of thermodynamics for a fixed-mass system (closed system)

$$\left.\frac{d\hat{E}_k}{dt}\right|_{system} = \frac{\delta Q_k}{dt} - \frac{\delta W_k}{dt}$$

The total energy includes internal, kinetic , potential, surface tension etc

For a control volume including only one phase *k, the energy equation for the control volume* can be obtained by setting the general property as $\Phi_k = E_k + m\mathbf{V}_{k,rel}^2/2$ and $\phi_k = e_k + \mathbf{V}_{k,rel}^2/2$

$$\left.\frac{dE_k}{dt}\right|_{system} = \frac{\partial}{\partial t}\int_V \rho_k\left(e_k + \frac{\mathbf{V}_{k,rel}^2}{2}\right)dV + \int_A \rho_k(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)\left(e_k + \frac{\mathbf{V}_{k,rel}^2}{2}\right)dA$$

E_k and e_k are, respectively, internal energy and specific internal energy. $\mathbf{V}_{k,rel}^2 = \mathbf{V}_{k,rel}\cdot\mathbf{V}_{k,rel}$

$$\frac{\delta Q_k}{dt} - \frac{\delta W_k}{dt} = \frac{\partial}{\partial t}\int_V \rho_k\left(e_k + \frac{\mathbf{V}_{k,rel}^2}{2}\right)dV + \int_A \rho_k(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)\left(e_k + \frac{\mathbf{V}_{k,rel}^2}{2}\right)dA$$

Heat Flow is due to conduction, internal energy generation, radiation etc

$$\frac{\delta Q_k}{dt} = \int_A -\mathbf{q}_k''\cdot\mathbf{n}_k dA + \int_V q_k''' dV$$

$\mathbf{q}_k''$ is the heat flux vector at the control volume surface

q_k''' is the internal heat generation

$$\frac{\delta W_{k,s}}{dt} = -\int_A (\mathbf{n}_k\cdot\boldsymbol{\tau}_k')\cdot\mathbf{V}_{k,rel}dA$$

The work done by the body force is

$$\frac{\delta W_{k,b}}{dt} = -\int_V\left[\sum_{i=1}^{N}\rho_{k,i}\mathbf{X}_{k,i}\right]\cdot\mathbf{V}_{k,rel}dV$$

Work done by normal and shear stress on surface and by body force

Now let us take a look at the energy equation, okay. The energy equation is basically nothing but the first law of thermodynamics for a fixed mass system right, okay. So, what is the first law of thermodynamics, we did it in the first lecture it is nothing but the rate of change of energy of the system.

This energy includes the internal energy, kinetic energy, potential energy any surface tension or other such energy that can be there okay. Most of the time we are concerned with internal energy but it is nothing but the heat and the work transfer right, these are the other two terms. This is a typical first law right.

For a control volume that contains only one phase because that is the methodology that we are following we are defining it for one phase and then we are showing that what kind of, if we take it across multiple phases, what will happen? So, now the property function that we define in the last class is nothing but the energy plus this kinetic energy hit okay.

And the corresponding small Phi k is nothing but the intensive version of the same. Now if we substitute the value of Phi k in the governing equation right, the equation that we established. We see that the rate of change of energy within the system it looks very familiar to like a conservation equation.

It basically tells you the rate of change of energy within the control volume and whatever is the flux that is happening okay, across the control surfaces. So, these are basically the internal energy and the specific internal energy capital Ek and small ek right. So, substituting this over here where we are substituting where we are bringing in the qk and the wk term.

The same expression is kind of valid right, okay. So, here we are proposing something which is a little bit interesting that this particular term which is nothing but the heat transfer across the control surface right. That we are proposing that can happen due to two ways okay. One is basically due to the internal energy generation inside the control volume right.

The other one is basically the flux that is coming due conduction right okay. So, this qk double prime into nk dA is nothing but a conductor. It is like a heat flux vector at the control surface, control volume surface right. And qk triple prime is nothing but the internal heat generation right, in the case of work term, now if we look at the work term over here now.

This work term is nothing but the work done by the normal and the shear stress and by the body force right. So, we already saw in the momentum equation that there was shear stress and then there was body force and then there was normal stress. So, this is the nothing but the work done by all those forces.

So, naturally by the total stress or work done by the total stress is given by this okay. Similarly the work done by the body force is given by this okay. So, these are the two work related term body force and by the normal stress okay and by the shear stress on the control volume.

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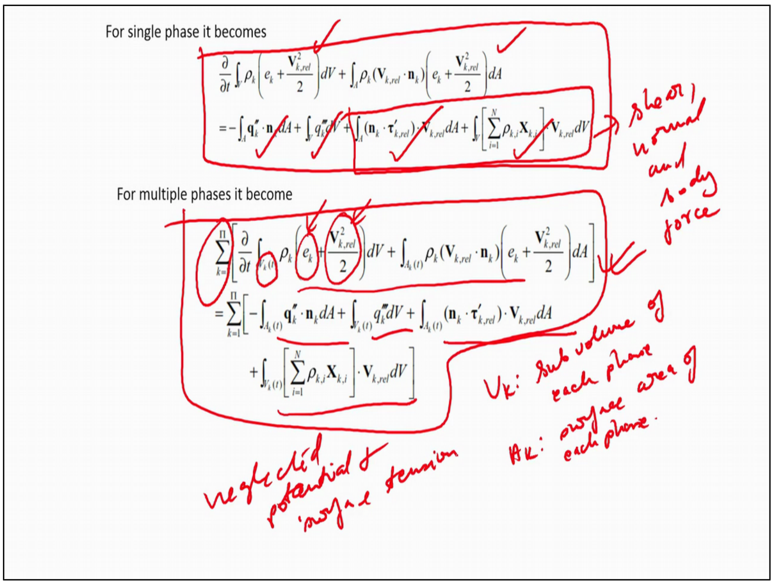

For single phase it becomes

$$\frac{\partial}{\partial t}\int_V \rho_k\left(e_k+\frac{\mathbf{V}_{k,rel}^2}{2}\right)dV+\int_A \rho_k(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)\left(e_k+\frac{\mathbf{V}_{k,rel}^2}{2}\right)dA$$
$$=-\int_A \mathbf{q}_k''\cdot\mathbf{n}_k dA+\int_V q_k''' dV+\int_A(\mathbf{n}_k\cdot\boldsymbol{\tau}_{k,rel}')\cdot\mathbf{V}_{k,rel}dA+\int_V\left[\sum_{i=1}^{N}\rho_{k,i}\mathbf{X}_{k,i}\right]\cdot\mathbf{V}_{k,rel}dV$$

shear, normal and body force

For multiple phases it become

$$\sum_{k=1}^{\Pi}\left[\frac{\partial}{\partial t}\int_{V_k(t)}\rho_k\left(e_k+\frac{\mathbf{V}_{k,rel}^2}{2}\right)dV+\int_{A_k(t)}\rho_k(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)\left(e_k+\frac{\mathbf{V}_{k,rel}^2}{2}\right)dA\right]$$
$$=\sum_{k=1}^{\Pi}\left[-\int_{A_k(t)}\mathbf{q}_k''\cdot\mathbf{n}_k dA+\int_{V_k(t)}q_k'''dV+\int_{A_k(t)}(\mathbf{n}_k\cdot\boldsymbol{\tau}_{k,rel}')\cdot\mathbf{V}_{k,rel}dA\right.$$
$$\left.+\int_{V_k(t)}\left[\sum_{i=1}^{N}\rho_{k,i}\mathbf{X}_{k,i}\right]\cdot\mathbf{V}_{k,rel}dV\right]$$

Vk: Sub volume of each phase

Ak: surface area of each phase.

neglected potential & surface tension

So, for a single phase there for assembling all these parts of the equation we get this final form okay. Now in this final form if you take a closer look you will find that once again the first two terms are basically your advective advection term or convective term okay. The first term on the right hand side designates your diffusion term or the conduction term right.

This is the internal energy generation term, this is basically the work done, these two are basically the work done component okay. By sheer normal stress and body force right, okay. For multiphase what we do we follow the same exercise, that we sum all these components right, across all the phases over here.

But with a special attention that this Vk is nothing but the individual sub volumes Vk is basically the sub volume of each phase. Similarly Ak is the surface area of each phase occupied by each phase okay. And basically we have summed over all the phases. So, that is the expression that you see.

So, the energy equation basically as we you already knew from your undergraduate is basically consists of the advection term, the conduction term, the heat generation term, the work that is done due to the shear stress and the normal stress and the work that is done by the body force okay. So, that is basically nothing but your energy equation right.

And this energy is basically the component sum together of the kinetic energy component and the internal energy component. And you can, here we have call of course neglected potential plus any surface tension related component, those we have neglected.

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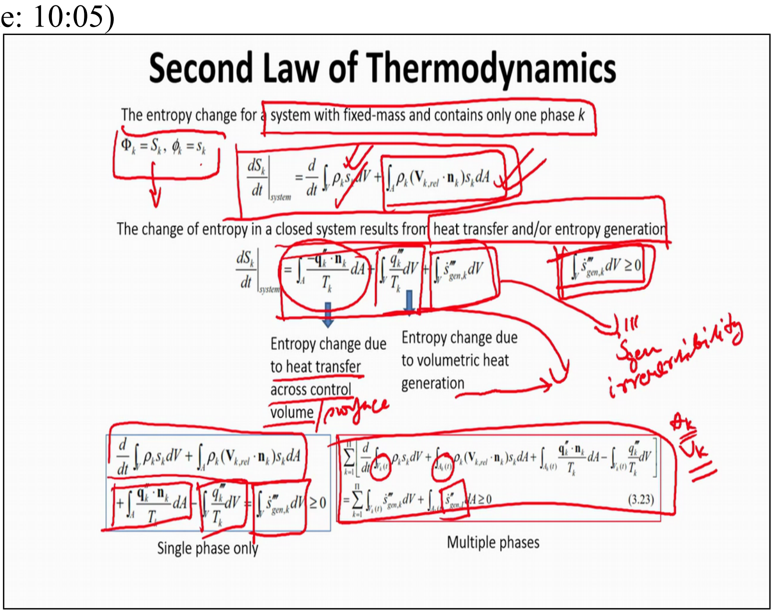

Second Law of Thermodynamics

The entropy change for a system with fixed-mass and contains only one phase k

$\Phi_k = S_k,\ \phi_k = s_k$

$$\left.\frac{dS_k}{dt}\right|_{system} = \frac{d}{dt}\int_V \rho_k s_k dV + \int_A \rho_k (\mathbf{V}_{k,rel}\cdot\mathbf{n}_k) s_k dA$$

The change of entropy in a closed system results from heat transfer and/or entropy generation

$$\left.\frac{dS_k}{dt}\right|_{system} = \int_A \frac{-\mathbf{q}''_k\cdot\mathbf{n}_k}{T_k}dA + \int_V \frac{q'''_k}{T_k}dV + \int_V \dot{s}'''_{gen,k}dV$$

$$\int_V \dot{s}'''_{gen,k}dV \geq 0$$

Entropy change due to heat transfer across control volume

surface

Entropy change due to volumetric heat generation

$\dot{s}'''$ gen irreversibility

$$\frac{d}{dt}\int_V \rho_k s_k dV + \int_A \rho_k(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)s_k dA + \int_A \frac{\mathbf{q}''_k\cdot\mathbf{n}_k}{T_k}dA - \int_V \frac{q'''_k}{T_k}dV = \int_V \dot{s}'''_{gen,k}dV \geq 0$$

Single phase only

$$\sum_{k=1}^{\Pi}\left[\frac{d}{dt}\int_{V_k(t)}\rho_k s_k dV + \int_{A_k(t)}\rho_k(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)s_k dA + \int_{A_k(t)}\frac{\mathbf{q}''_k\cdot\mathbf{n}_k}{T_k}dA - \int_{V_k(t)}\frac{q'''_k}{T_k}dV\right]$$
$$= \sum_{k=1}^{\Pi}\int_{V_k(t)}\dot{s}'''_{gen,k}dV + \int_{A_k(t)}\dot{s}''_{gen,I}dA \geq 0 \quad (3.23)$$

Multiple phases

A_k

V_k

Moving on, so, we have done basically the conservation of energy, conservation of mass, conservation of momentum. Now let us look at the second law of thermodynamics right, applied to a system with fixed mass and containing one phase only because that is how we start. Here of course the variable, the property is basically nothing but the kinetic energy of the kth phase, right.

So, this is the extensive quantity, this is the intensive quantity okay. So, how do we write it, once again the same expression is valid right. The rate of change of entropy in the system is given by the trait of entropy within the control volume plus whatever is the entropy that is coming out, right, through the control surfaces right, okay.

So, that changes of entropy in a closed system results from heat transfer and or odd entropy generation correct. So, the entropy change in the system happening due to heat transfer is given by this expression. The entropy change due to the heat generation is given by that expression and then there is of course the entropy generation term okay. Itself!

So, what is this particular term this is essentially the heat transfer across the control volume or control surface okay. This is basically nothing but the entropy generation due to volumetric heat. And this is the normal entropy generation term which has to be greater than 0 basically. This is dot triple gen okay.

Now for a single phase therefore if we put all these parameters together you will once again have that there is a convective term okay, there is a entropy that is generated or the entropy that change that happens due to the heat transfer across the control surface entropy that is generated due to volumetric heat generation.

And this expresses the extent of the irreversibility right. So, there is an entropy generation in the control volume, so, this entire thing is greater than zero that is because the generation term is actually greater than zero, right. You do it for multiple phases it is the exact same expression that we have, okay.

Once again only thing that is taken care of is Ak and Vk, Ak and Vk these are the only two things that you need to take care right. So, whenever you do you are doing it for the particular sub volume and the sub control surfaces essentially right. And you are summing them together and you are coming the entropy that is generated in each of the phases okay.

And then you show that this has to be great an equal to 0, right. So, this is basically the second law of thermodynamics when you cast it in a control volume approach okay. I think it should be pretty clear, right. There is always a rate of change of that particular variable inside; of that property inside the control volume and then there is a flux term.

These are the two universal thing okay. Now in addition to that we are stating that this should be related the entropy change is also related to the change of due to heat transfer heat generation and the normal generation because of the irreversibility of the process. This is due to irreversibility okay. So, that is what this particular term is.

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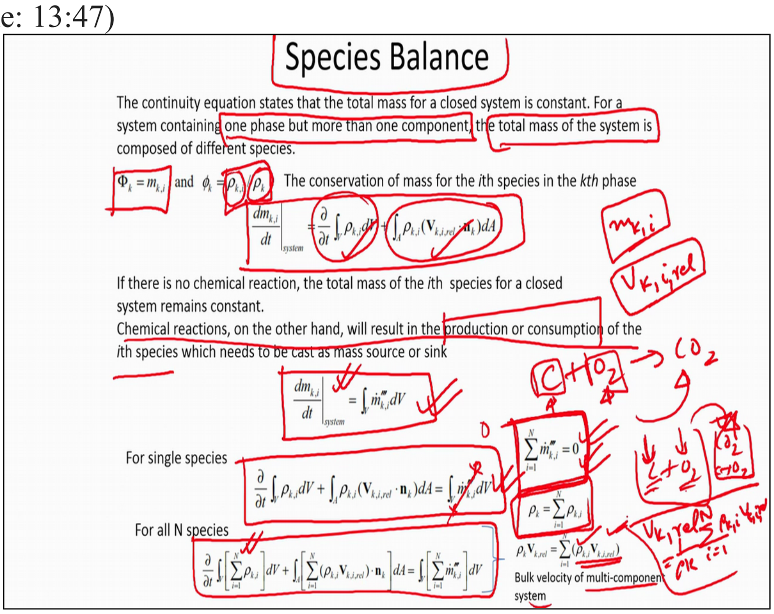

Species Balance

The continuity equation states that the total mass for a closed system is constant. For a system containing one phase but more than one component, the total mass of the system is composed of different species.

$\Phi_k = m_{k,i}$ and $\phi_k = \rho_{k,i}/\rho_k$ The conservation of mass for the *i*th species in the *kth* phase

$$\left.\frac{dm_{k,i}}{dt}\right|_{system} = \frac{\partial}{\partial t}\int_V \rho_{k,i}\,dV + \int_A \rho_{k,i}(\mathbf{V}_{k,i,rel}\cdot\mathbf{n}_k)\,dA$$

If there is no chemical reaction, the total mass of the *i*th species for a closed system remains constant.

Chemical reactions, on the other hand, will result in the production or consumption of the *i*th species which needs to be cast as mass source or sink

$$\left.\frac{dm_{k,i}}{dt}\right|_{system} = \int_V \dot{m}'''_{k,i}\,dV$$

For single species

$$\frac{\partial}{\partial t}\int_V \rho_{k,i}\,dV + \int_A \rho_{k,i}(\mathbf{V}_{k,i,rel}\cdot\mathbf{n}_k)\,dA = \int_V \dot{m}'''_{k,i}\,dV$$

For all N species

$$\frac{\partial}{\partial t}\int_V\left[\sum_{i=1}^{N}\rho_{k,i}\right]dV + \int_A\left[\sum_{i=1}^{N}(\rho_{k,i}\mathbf{V}_{k,i,rel})\cdot\mathbf{n}_k\right]dA = \int_V\left[\sum_{i=1}^{N}\dot{m}'''_{k,i}\right]dV$$

$$\sum_{i=1}^{N}\dot{m}'''_{k,i} = 0$$

$$\rho_k = \sum_{i=1}^{N}\rho_{k,i}$$

$$\rho_k\mathbf{V}_{k,rel} = \sum_{i=1}^{N}(\rho_{k,i}\mathbf{V}_{k,i,rel})$$

Bulk velocity of multi-component system

Now we look at the final thing which is nothing but the species balance equation okay. Species balance, why the species balance is important because species balance equation as I said, if it is a single component system it does not really matter okay. But if it is a system which is a reacting system like for example a combusting system or any other similar type of system, species actually do play a major role, right, okay.

So, if the system contains one phase and more than one component that for how we start, single-phase multi component system, the total mass of the system is composed of multiple species, correct. Because it may be add nitrogen CO2 there may be thousands of species that may be present. There is no limitation as to the total number of species that that can be there okay.

So, here the Phi k, now that we define is basically nothing but the mass of the ith species in the kth phase okay. So, this mask m ki is basically the mass of the ith species in the kth phase. So, say for example is water that means it is the mass of water in whatever phase it is presenting in. Then there can be air. So, it can be mass of air in whatever phase it is presented okay.

So, similar thing when you and actually a small Phi k is nothing but the variation in the density. This is the density of the ith component in the kth phase okay. And this is the total density or the average density okay. So, now when we write the change of mass of the ith component in the kth phase in that particular system.

Once again it is composed of two components, right. So, one is the rate of change of that particular component within the control volume the other one is a flux term, right. Remember here the velocity is V ki relative that means this is the velocity of the ith species in a kth phase. This is a relative velocity basically of the ith species in the kth phase, okay.

And this Rho ki is nothing but the density of the ith species in the kth phase, okay. So, if there is no chemical reaction for example, okay. The total mass of the ith species remains constant, right. So, it is exactly like a continuity equation right because if there is no reaction say for example in a vessel okay, you have water vapour, air, co2, nitrogen everything you have put together like this room for example okay.

This is a multi component system room but here you do not have any chemical reaction right. So, if you do not have any chemical reaction the total mass of the ith species remains constant right. So, species wise okay it is almost like a mass conservation. Chemical reactions on the other hand if it happens it lead to the production and consumption of ith species, right.

Say for example if you have a reaction C and C plus O2 and form CO2, right. What happens is that there were two components C and O O2, they are consumed and you create CO2 in its place right. The total mass is still conserved right, the total mass is still conserved that we already know. But individually the species mass are not conserved okay.

So, the C and the O2 if this is a vessel which initially had C plus O2 okay after some time you will get the same vessel where there will be lot of CO2 and very little C and O2. It will be still there but it will be very quantities, right. So, if you started with one gram of C and one gram of O2 you might end up getting a .1 gram of C and .1 gram O2 or something like that okay.

Because the rest has been converted to CO2 the mass is still conserved okay but the mass of the individual species are not. So, it leads to production and consumption of the ith species which needs to be cast as a mass source or sink term okay. Like for example take a look at this particular equation over here right.

So, this is the rate of change of mass okay of the ith species in the kth state in the system and that can only be given by some kind of a sink or source term. This m triple prime ki dV is nothing but a sink or a source. It can be a depletion it can be a production also right. So, for a single species it looks very familiar to a mass conservation equation except that in the mass conservation equation this term basically goes to zero.

But here in this case obviously you are not going to have that okay taking into account chemical reaction; you produce mass within the control volume, rate of mass production within the control volume okay. But note one other thing the rate of production or consumption of mass of the ith species and I mean all the species combined has to be equal to zero because globally the mass has to be conserved, right.

So, say for example here see the concentration of C and the mass of C and the mass of O2 may be coming down. But the mass of CO2 actually increases correct, mass of CO2 increases the mass of C and O2 actually drops, okay. So, here what we can see is that the rate of production or consume; the total rate of production or consumption of mass is basically zero, okay.

And one other thing is that the density, the total density is nothing but the sum total of all the density of all the individual components or the individual species right. So, for all the N species you just need to come together this expression with correspondingly over N. N is the total number of species not the number of phases though.

And this Vk relatives which is the relative velocity or the bulk relative velocity of a multi-component system is nothing but the density waited okay. It is that density waited is it Rho k into Vk right. So, it is the density we waited summation of all the individual species of the system right.

So, that is why that Vk can be written as 1 over Rho k, okay, summation of i =1 to N Rho ki into Vki relative, right. So, that you can say from this particular expression right, so, it is nothing but the density average velocity of each of the component. So, that is the species balance in a nutshell right.

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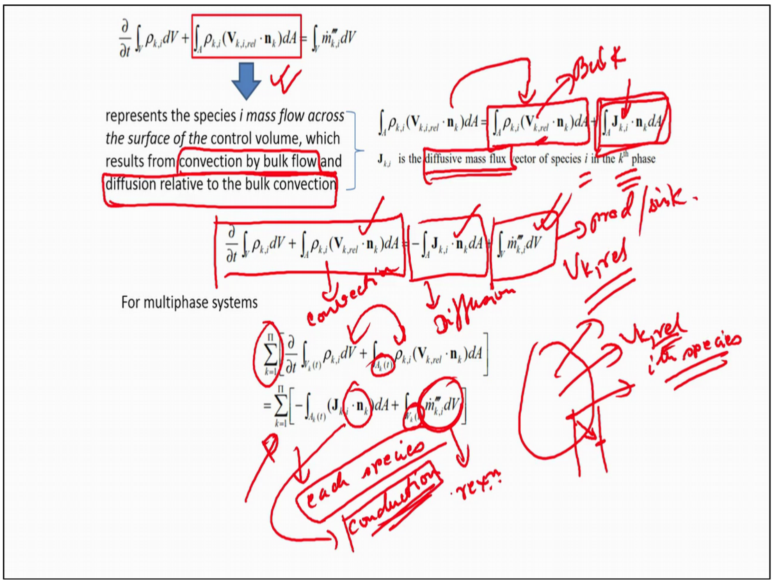

$$\frac{\partial}{\partial t}\int_V \rho_{k,i}dV + \boxed{\int_A \rho_{k,i}(\mathbf{V}_{k,i,rel}\cdot\mathbf{n}_k)dA} = \int_V \dot{m}'''_{k,i}dV$$

represents the species *i mass flow across the surface of the* control volume, which results from convection by bulk flow and diffusion relative to the bulk convection

$$\int_A \rho_{k,i}(\mathbf{V}_{k,i,rel}\cdot\mathbf{n}_k)dA = \boxed{\int_A \rho_{k,i}(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)dA} + \boxed{\int_A \mathbf{J}_{k,i}\cdot\mathbf{n}_k dA}$$

$\mathbf{J}_{k,i}$ is the diffusive mass flux vector of species i in the k^{th} phase

$$\boxed{\frac{\partial}{\partial t}\int_V \rho_{k,i}dV + \int_A \rho_{k,i}(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)dA} = \boxed{-\int_A \mathbf{J}_{k,i}\cdot\mathbf{n}_k dA} + \boxed{\int_V \dot{m}'''_{k,i}dV}$$

For multiphase systems

$$\sum_{k=1}^{\Pi}\left[\frac{\partial}{\partial t}\int_{V_k(t)} \rho_{k,i}dV + \int_{A_k(t)} \rho_{k,i}(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)dA\right] = \sum_{k=1}^{\Pi}\left[-\int_{A_k(t)}(\mathbf{J}_{k,i}\cdot\mathbf{n}_k)dA + \int_{V_k(t)} \dot{m}'''_{k,i}dV\right]$$

Now if you look at this particular expression over here it is not complete yet. Say the second term on the left-hand side okay, this represents the species i mass flow across the surface of the control volume which resolves which can result from convection of the bulk flow as well as diffusion with respect to the bulk conviction.

So, one can be due to bulk convection right okay across the control surface. So, species i move across the control surface that may be due to the velocity that it carries by itself, right. It could be also because of the diffusion on the top of that bulk convection is not that so. So, if you write these expressions you will find that there is a component which is Vk relatives that is the relative component with the movable relative velocity.

That is the kth velocity okay, so, that is like the bulk, this is the bulk right. And there is another component which is given by that J, J is basically the diffusive mass flux vector of species i in the kth phase okay. To understand this basically what we have done is that we have said that the species is getting transported across the control surface, right. Good thing;

Now this transport of species across the control surface may be happening due to the convection of the bulk flow. Bulk flow is Vk a relative, so, this bulk flow carries with it okay, a certain amount of species. So, this is a control volume there is a bulk flow that is going out which is given by Vk relative, right.

So, as it is flowing out it is carrying the ith species with it, right. But on the top of that if there are concentration gradients across the flow feet, right. It can happen right, so, from here say for example the concentration of species i is higher than here, right. So, there will be a diffusive transport okay.

It is like a conduction problem that means when there is a temperature gradient there is a heat flow here when there is a concentration gradient there is a corresponding species flow. That is not the bulk flow that we are talking about over here okay. So, that is given by this J okay. So, the diffusive mass plus vector, so, now what we have is basically, we have a convective derivative fully.

We have a diffusion term and we have a corresponding production term. This is diffusion this exactly looks like a heat balance equation, this is the basically the convection. Convection, advection whatever you call it and this is basically production or sink kind of vector. Now for multiphase systems what we do is basically we for each species, this is for each species, right.

So, each species may be present in 2, 3 in at least two phases. So, there if sum total it over each of the individual phases right, once again Ak the Vk comes into the picture, right. So, this is nothing it all remains the same except that okay, we are having a transport of the each species as per this particular equation, right.

So in a multi-component system that is what happened this is the term that it is only reserved for reaction basically got it. So, I think in this particular slide what we have explained over there is that you not only have a convection but you also have a diffusion of species because you can have a concentration gradient.

Because there are many species that are present in the system and you also can have a production or a destruction kind of a term of the species okay. And you have the similar this looks exactly the same like a mass balance equation like a continuity equation only this term is new and this term is new. But this term looks familiar to a heat conduction equation it looks very familiar to a heat conduction equation, right.

Look very, very familiar to a heat conduction term right that you have in the energy equation, right. At the same time okay, so, this heat conduction equation is like it is very similar to heat conduction except that instead of temperature gradient you have a species balance gradient over here, okay. So, this completes the species balance part of the thing.

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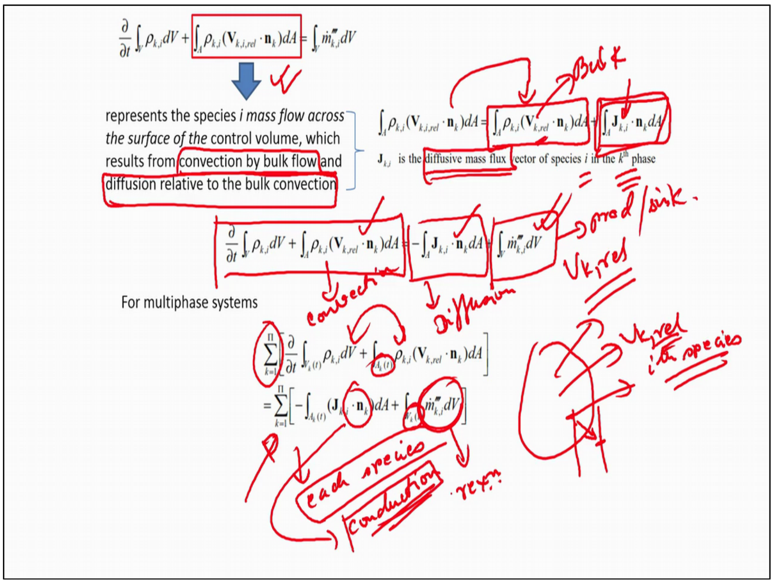

$$\frac{\partial}{\partial t}\int_V \rho_{k,i}dV + \boxed{\int_A \rho_{k,i}(\mathbf{V}_{k,i,rel}\cdot\mathbf{n}_k)dA} = \int_V \dot{m}'''_{k,i}dV$$

represents the species *i mass flow across the surface of the* control volume, which results from convection by bulk flow and diffusion relative to the bulk convection

$$\int_A \rho_{k,i}(\mathbf{V}_{k,i,rel}\cdot\mathbf{n}_k)dA = \int_A \rho_{k,i}(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)dA + \int_A \mathbf{J}_{k,i}\cdot\mathbf{n}_k dA$$

$\mathbf{J}_{k,i}$ is the diffusive mass flux vector of species i in the k^{th} phase

$$\frac{\partial}{\partial t}\int_V \rho_{k,i}dV + \int_A \rho_{k,i}(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)dA = -\int_A \mathbf{J}_{k,i}\cdot\mathbf{n}_k dA + \int_V \dot{m}'''_{k,i}dV$$

For multiphase systems

$$\sum_{k=1}^{\Pi}\left[\frac{\partial}{\partial t}\int_{V_k(t)} \rho_{k,i}dV + \int_{A_k(t)} \rho_{k,i}(\mathbf{V}_{k,rel}\cdot\mathbf{n}_k)dA\right] = \sum_{k=1}^{\Pi}\left[-\int_{A_k(t)} (\mathbf{J}_{k,i}\cdot\mathbf{n}_k)dA + \int_{V_k(t)} \dot{m}'''_{k,i}dV\right]$$

Now in most of the time we basically a deal with instead of integral formulation, we deal with differential formulations, right, because differential formulations are sometimes easier to handle. Now all of these can be derived from the integral formulation as well. Now for the differential formulation it is necessary first to apply the divergence theorem.

What is the divergence theorem? This is basically any property that you can think of okay. So, that property okay, which is enclosed by a control volume a control for; this is a control volume V which is basically enclosed by a piecewise smooth control surface. So, basically what we can do is that this area integral can be converted to the corresponding volume integral, right.

So, this is nothing but the flux of whatever is the quantity that you are dealing with right, with respect to the surface normal okay, of the enclosed area. Now if it is piecewise smooth okay, then this is related to the divergence of the same component okay, in the on the on a volume basis, right. And furthermore since the control volume shape and size are fixed in space we can apply let this rule okay for any specific general quantity.

And we can say that this is the formulation this, let me through you have seen in the case of your boundary layer analysis also right. So, it says that if it is control volume is fixed shape and size are fixed in time right we can cast the rate of change of whatever is the property over here and we can take this basically within this integral sign okay.

So, the conservation of mass basically what does it become initially this was the, this is, these are the two reduction terms like for example the flux term in the case of conservation of mass that is the flux term across the control surface is now converted to the corresponding divergence, right.

The divergence of this particular quantity right and what will happens is that if we apply now, okay, this transformation everything now is on a volume basis, right. The integral now becomes only with respect to volume there is no area if you just quickly take a look what we did earlier.

You will find that here for example take a look at this particular expression right here we see that there is an area basis right. And this is the one that is run the volume basis. Now what we have done in this particular case is basically we have converted that area integral to a volume integral, correct, using the divergence theorem, right.

And we have taken now and then using Leibniz's rule, we convert the continuity equation to this particular form, correct, okay. So, for now if you see this integral is basically equal to 0. Now since it is valid for any arbitrary shape and size that means you can shrink the control volume okay with impunity to as small a size as you want, right.

Then the integrand must be also equal to 0, right that is the integrand must be also equal to 0 because it is valid for any control volume right no matter how small or how large it is, right. So, integrand equal to 0 means this particular term becomes equal to 0, right. So, this is the standard continuity equation that you may have seen in your undergraduate or first-level graduate courses, okay.

So, this can be basically written by a material derivative okay, D Rho k by Dt plus this divergence component right. So, this is basically by the divergence of velocity that we have right. So, it is basically this D by DT is basically nothing but the material derivative as I said just now. It is composed of the time derivative as Vk relatives into the corresponding operator right.

So, these acts on the density right now if it is an incompressible flow say for example that things the density does not change.
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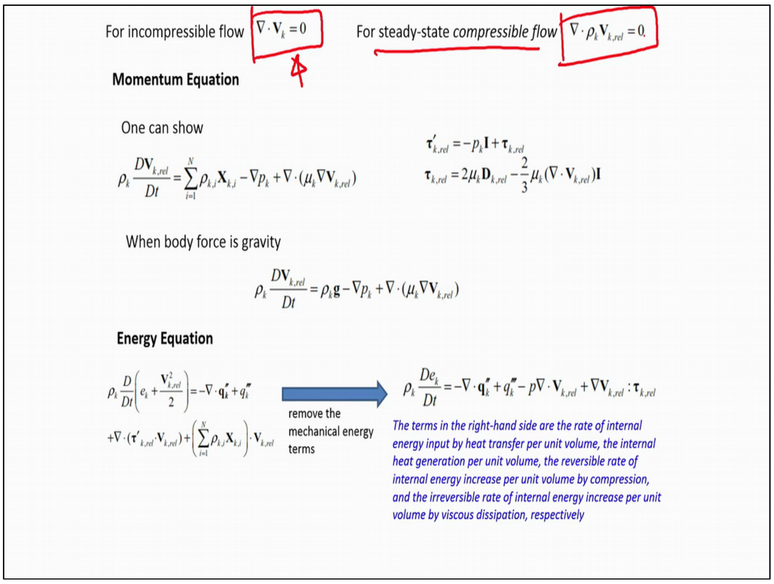

For incompressible flow $\boxed{\nabla \cdot \mathbf{V}_k = 0}$ For steady-state *compressible flow* $\boxed{\nabla \cdot \rho_k \mathbf{V}_{k,rel} = 0}$

Momentum Equation

One can show

$$\rho_k \frac{D\mathbf{V}_{k,rel}}{Dt} = \sum_{i=1}^{N} \rho_{k,i} \mathbf{X}_{k,i} - \nabla p_k + \nabla \cdot (\mu_k \nabla \mathbf{V}_{k,rel})$$

$$\boldsymbol{\tau}'_{k,rel} = -p_k \mathbf{I} + \boldsymbol{\tau}_{k,rel}$$

$$\boldsymbol{\tau}_{k,rel} = 2\mu_k \mathbf{D}_{k,rel} - \frac{2}{3}\mu_k (\nabla \cdot \mathbf{V}_{k,rel})\mathbf{I}$$

When body force is gravity

$$\rho_k \frac{D\mathbf{V}_{k,rel}}{Dt} = \rho_k \mathbf{g} - \nabla p_k + \nabla \cdot (\mu_k \nabla \mathbf{V}_{k,rel})$$

Energy Equation

$$\rho_k \frac{D}{Dt}\left(e_k + \frac{\mathbf{V}_{k,rel}^2}{2}\right) = -\nabla \cdot \mathbf{q}''_k + q'''_k + \nabla \cdot (\boldsymbol{\tau}'_{k,rel} \cdot \mathbf{V}_{k,rel}) + \left(\sum_{i=1}^{N} \rho_{k,i} \mathbf{X}_{k,i}\right) \cdot \mathbf{V}_{k,rel}$$

remove the mechanical energy terms

$$\rho_k \frac{De_k}{Dt} = -\nabla \cdot \mathbf{q}''_k + q'''_k - p\nabla \cdot \mathbf{V}_{k,rel} + \nabla \mathbf{V}_{k,rel} : \boldsymbol{\tau}_{k,rel}$$

The terms in the right-hand side are the rate of internal energy input by heat transfer per unit volume, the internal heat generation per unit volume, the reversible rate of internal energy increase per unit volume by compression, and the irreversible rate of internal energy increase per unit volume by viscous dissipation, respectively

We only get the divergence of velocity to be equal to 0, right. So, that is not that is why in many of the problems that you solve you find that the divergence of velocity is always equal to 0 for incompressible flow. However for steady-state compressible flow is not the divergence of velocity but the divergence of this that is actually equal to 0, right, okay.

So, this shows that how easily we can convert an integral formulation to a corresponding differential formulation just by using the divergence theorem and the Lebniz's rule okay, nothing else, okay. So, in the next class what we are going to do is that we are going to take a look now at the momentum equation okay.

So, we will stop here and we start in the start in the next lecture when we look at the differential formulation of the momentum equation.