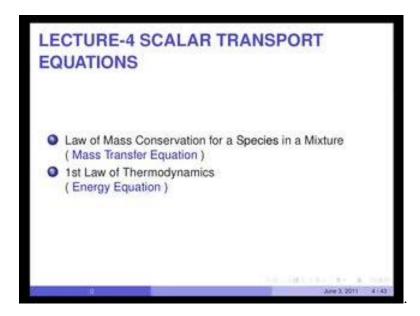
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# Module No. # 01 Lecture No. # 04 Scalar Transport Equations

In the last lecture, we saw equations of fluid motion namely the law of mass conservation applied to the bulk fluid as well as the second law of motion also called the Navier-Stokes equations.

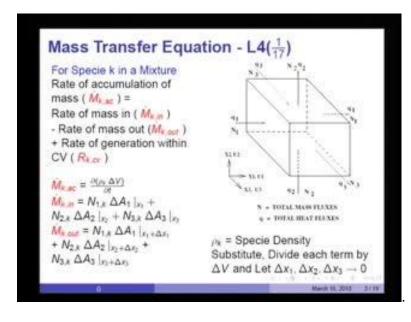
Moving fluids also carry with them scalar quantities. Today, we are going to look at equations that govern transport of scalar quantities.

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The first scalar quantity is the specie in a mixture. For example, if you are dealing with a combustion problem then the species carried are oxygen, carbon dioxide, fuel, carbon monoxide and so on and so forth.

The law of mass conservation for a specie in a mixture is called the mass transfer equation. We will also invoke the first law of thermodynamics which transports energy in a moving fluid. Both energy and the concentration of the specie are scalar quantities.



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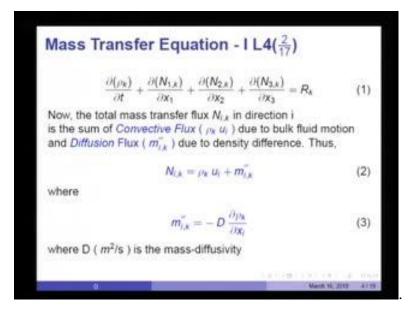
What does the law say for a specie? For a specie k in a mixture, the rate of accumulation of mass of the specie k that is given by M dot k accumulation equals rate of mass in minus rate of mass out plus rate of generation of specie within the control volume.

As a result of chemical reaction, as you know some species are generated and while others are destroyed. As such each specie will have either a generation or a destruction rate associated with it. What is M dot k accumulation? That is simply the mass of the specie k within the control volume delta v - d by dt of rho k delta v.

The mass of specie in will be the flux of specie k in direction 1 multiplied by the area d A 1 which is this area plus N 2 k which is coming from the bottom multiplied by the area delta A 2 plus N 3 k multiplied by delta A 3 at x 3 and likewise the same quantities at the outgoing phases at x1 plus delta x 1, x 2 plus delta x 2 and x 3 plus delta x 3; rho k is the specie density.

If we now substitute these expressions in this verbal statement and divide each term by delta v which is the product of delta x 1, delta x 2 and delta x 3 and let each of these increments tend to 0; this is a procedure we have gone through before.

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Then you will see you will get an equation of this type d rho k by dt plus net transport of specie k in direction 1, plus net transport in direction 2, plus net transport in direction 3 equal to rate of generation of specie k.

Now, the total mass flux N i k in direction i is the sum of the convective flux due to rho k u i due to bulk fluid motion and diffusion flux m double prime i k due to density difference. Thus N i k is represented as rho k u i plus m double dot i k.

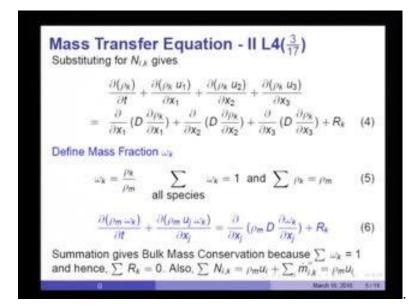
Writing convective flux in this manner is indicative of the fact that we are assuming that each specie is traveling or is being carried at the same velocity as the bulk fluid. The diffusion flux on the other hand m double dot i k arises simply due to the differences in density at neighbouring locations.

The expression for mass flux by diffusion is given as m double prime i k equal to minus D rho k by d x i. This equation is analogous to the conduction heat transfer and is like a Fourier's law of heat conduction.

In mass transfer, it is called the fix law of mass diffusion. So, just as in convective heat transfer you know that the total flux of energy is given by the convecting flux plus conduction flux. In mass transfer, we say it is the convective flux plus diffusion flux.

D is called the mass-diffusivity; it has units of meter square per second. So, if I have to substitute for N i k for each of these terms then I can rewrite this equation in the following manner.

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It would read as d rho k by dt plus d rho k u 1 by d x 1 and so on and so forth is equal to  $\frac{d}{d} \frac{d}{d} \frac{d}{d}$ 

Rho k has units of density. It is customary to define mass fraction omega k as the specie density divided by the mixture density and therefore, sum sigma omega k equals 1 by Dalton's law. Another way of saying is sum of densities is equal to the mixture density.

The notion behind Dalton's law is that each specie behaves as though it occupies the volume of the total mixture.

If I were to substitute now, rho k as rho m multiplied by omega k, this equation would be written in tensor notation in this fashion this is called the mass transfer equation. It has a transient term, a convection term, a diffusion term and a source or a generation term.

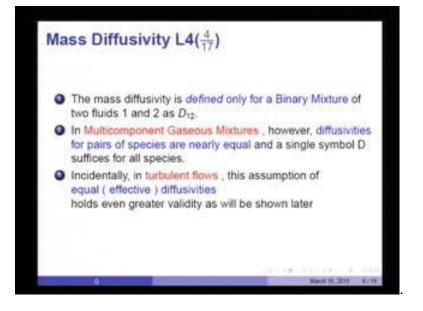
Now, let us sum each of these terms over all species - that is sum over all k as done here. (Refer Slide 07:38) Then clearly here this term would reduce to d rho m by d t; this term would reduce to d rho m u j by d x j because omega k is equal to 1.

Sigma omega k will simply become unity or constant. Therefore, this term would simply vanish. Just see now that this equation would be d rho m by d t plus d rho m u j by d x j equal to sigma R k and that term is here. You will recognize readily then in the absence of omega k, the left hand side is simply the bulk mass conservation and it equals 0; it follows therefore the sigma R k must be 0.

These two last deductions are very important. sigma R k equal to 0 says that whenever there is a chemical reaction it is true that some species will be generated, but there would be others that would be destroyed and the total mass cannot be generated or destroyed; that idea is expressed in sigma R k equal to 0.

What does summation of diffusion equal to 0 imply? It implies that when some species are being diffused in a certain direction, other species are being diffused in the opposite direction and that stands to reason.

For example, if fuel was decreasing then product would increase. The net result is that summation of all diffusive quantities would be 0 and therefore, sigma N i k would be sigma rho m u i plus sigma m double prime i k, but that quantity is 0 and therefore, sum of the mass fluxes in direction i are simply the bulk mass flux rho m u i. We shall refer to this equation much later in the course.



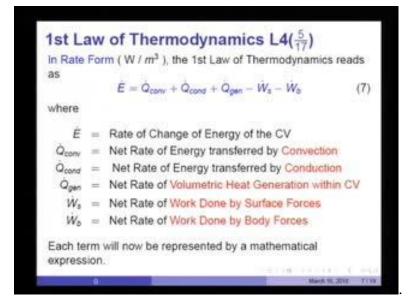
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A word about Mass Diffusivity: strictly speaking mass diffusivity is defined only for a Binary Mixture of two fluids 1 and 2 as D 1 2.

But in a combusting product mixture for example, there are several species present and diffusivities of pairs of species are truly different. So, diffusion of carbon dioxide in nitrogen or the diffusivity of carbon dioxide in nitrogen is different from diffusivity of oxygen in nitrogen and vice versa, but in gaseous mixtures these diffusivity pairs between species tend to be very nearly equal and therefore, we discard D 1 2 or d i j as the symbol for diffusivity and replace it by single symbol D and that suffices for combustion calculations.

Incidentally in turbulent flow, this assumption of equal effective diffusivity holds even greater validity; this we shall appreciate a little later.

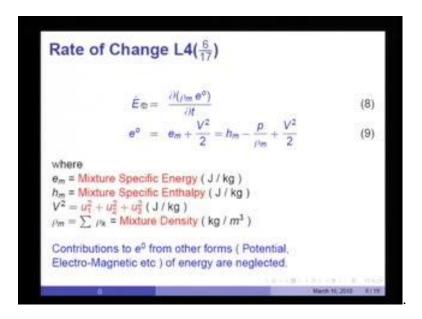
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We now turn to the first law of thermodynamics in rate form that is Watts per cubic meter. The first law of thermodynamics reads as d E by d t equal to d Q convection by d t plus d Q conduction by d t plus rate of generation of energy minus work done by shear forces minus work done by body forces.

Each of these terms is defined here and we shall seek mathematical representations for each one of them.

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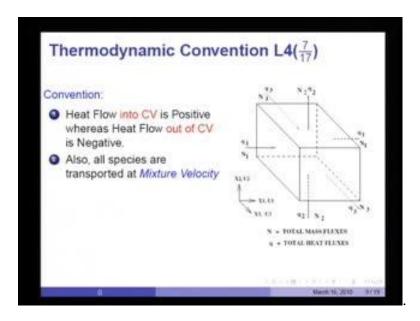
So, let us consider the first term E dot; that would simply be d by d t rho m e naught or the total energy. The total energy is the sum of static energy plus kinetic energy and the static energy by a thermodynamic relation is nothing, but enthalpy minus p into specific volume or p divided by rho m plus V square by 2.

So, e m is mixture specific energy, h m is mixture specific enthalpy, V square is the kinetic energy - sum of u 1 square, u 2 square and u 3 square and rho m as we saw before is sigma rho k, the Mixture Density.

In general, e naught will have contributions from many other force effects like potential energy associated with rise or fall in elevation, electro-magnetic energies and so on and so forth, but these we will neglect because practical equipment's are fairly small.

But in which Yes, kinetic energy would be of some interest, but not these energies that I mentioned at the moment.

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Now, in order to represent the heat transfer and the work transfer across a control volume we shall follow the thermodynamic conventions. We will say that heat flow into the control volume is positive whereas, the heat flow out of the control volume is negative.

As we said before, all species are transported at mixture velocity. Here, I have shown all the net mass transfers and heat transfers that could take place across a control volume phase. N is total mass flux and q is the total heat flux across the control volume phase.

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Net Convection L4(
$$\frac{\vartheta}{17}$$
)  
Since  $\sum N_{l,k} = \rho_m u_l$   
 $\hat{Q}_{conv} = -\frac{\partial \sum (N_{l,k} \theta_k^o)}{\partial x_l} = -\frac{\partial}{\partial x_l} \left[ (\sum N_{l,k} h_k) + \rho_m u_l (-\frac{p}{\rho_m} + \frac{V^2}{2}) \right]$   
(10)  
Now, following definition of  $N_{l,k}$  and noting  $\sum \omega_k h_k = h_m$ ,  
 $\sum N_{l,k} h_k = \sum (\rho_m u_l \omega_k + m_{l,k}^c) h_k$   
 $= \rho_m u_l h_m + \sum m_{l,k}^c h_k$  (11)  
Hence, after some algebra  
 $\hat{Q}_{conv} = -\frac{\partial (\rho_m u_l \theta^o)}{\partial x_l} - \frac{\partial (\sum m_{l,k}^c h_k)}{\partial x_l}$  (12)

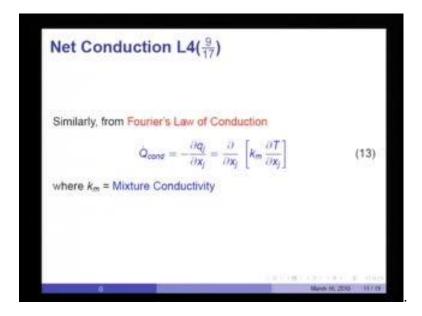
Net convection then by following the convention that the heat in is positive whereas, heat out is negative, we would have convection as simply d by d x j of sigma N j k e naught k and if I replace e naught k by h k minus p by rho m plus V square by 2.

Then you will see N j k would multiply with h k into the bracket, but the sum of N j k would simply be rho m u j as we saw before minus p by rho m plus V square by 2. If we now note that omega k into h k, that is the mass fraction of specie k multiplied by its specific enthalpy must add up to the mixture enthalpy; then sigma N j k h k would be sigma rho m u j omega k plus m double dot j k, the diffusion flux into h k.

Since sigma omega k h k is equal to h m, it will add up to rho m u j h m plus sigma m double prime j k h k.

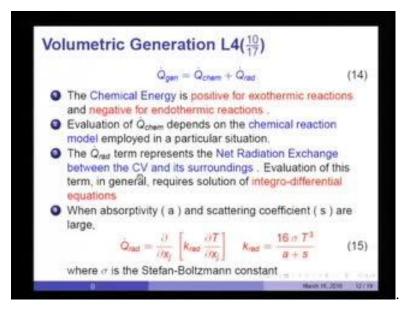
(Refer Slide Time: 15:37) Therefore, if I replace this term here then you will see you have rho m u j h m minus p by rho m plus V square by 2 which would be written in this fashion and then the left over term, the diffusion flux term that could be given by that term. So, that is the expression for the convective flux.

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Net conduction again by Fourier's law of conduction: Q conduction will be simply minus d q j by d x j where q j is k m multiplied by d T by d x j and k m is the mixture conductivity.

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Net volumetric generation: Now, volumetric generation in a moving fluid typically would comprise of the generation due to chemical energy because some reactions are exothermic whereas, some other chemical reactions are endothermic. So, Q dot chem would be positive in case of exothermic reactions and it would be negative in terms of endothermic reaction.

If you want to evaluate Q dot chem in a moving fluid then one needs to postulate first of all the chemical reaction model that is being employed and there are variety of chemical reaction mechanisms of different levels of complexity. We shall see all these when we come to study of mass transfer.

Q rad represents the net radiation exchange between the control volume and its surroundings. Usually evaluation of this term would require what is called the radiation transfer equation and it happens to be an integro-differential equation.

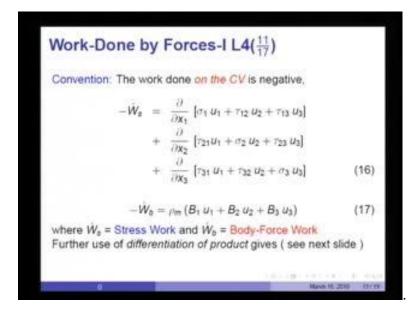
Treatment of that equation is really beyond the scope of the present lectures and it would require usually numerical calculations in a real practical equipment, but suppose the mixture that we are carrying has very high absorptivity may be because of soot, may be because of particulates that are present in the gaseous mixture.

Then the absorptivity and scattering of the radiation would be very high. When absorptivity and scattering coefficients are large, Q dot rad can actually be represented in

a manner similar to the conduction equation. The radiation conductivity can be defined as 16 into sigma T cube divided by a plus s where sigma is the Stefan-Boltzmann constant that you are all familiar with.

But remember this kind of representation is justified only when the gaseous mixture has very high absorption and scattering coefficients.

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Now, we come to the work done terms and the derivation to follow is somewhat longish and I would request you to play good attention to how the derivation progresses.

Firstly there are shear forces and normal forces. Here is the stress; stress is force per unit area multiplied by velocity gives you the work done and d by d x 1 of that gives you the net work done.

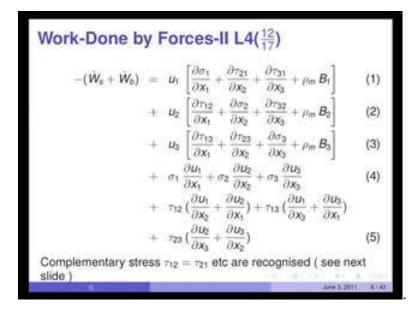
So, sigma 1 which acts in the direction 1 multiplied by u 1 plus tau 1 2 into u 2 is the work is the shear work in net shear work in x 1 direction and so on and so forth.

You will get shear stress multiplied by the associated velocity in the two directions and the net work done by stresses W dot s would be given as that.

The body forces work is rho m into B 1, the force multiplied by the velocity u 1 is the work done in direction 1, 2 and 3 likewise. So, W dot s is the stress work; W dot B is the Body-Force Work.

Now we shall write these things as differentiation of a product. So, this d by d x 1 sigma 1 u 1 will be written as sigma 1 d u 1 by d x 1 plus u 1 into d sigma 1 by d x 1 and so on and so forth.

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On the next line you will see the result. So, the total work-done will be u 1 multiplied by all these terms, u 2 multiplied by all these terms, u 3 multiplied by all these terms, plus sigma 1 d u 1 by d x 1, sigma 2 d u 2 by d x 2, sigma 3 d u 3 by d x 3, tau 1 2 into the strain rate associated with tau 1 2, tau 1 3 into the strain rate associated with tau 1 3, and tau 2 3 into the strain rate associated with tau 2 3 and here I have already used the idea of complementarities of stresses that is tau 1 2 is equal to tau 2 1. Now I draw your attention to this term.

If you recall, when we wrote the Navier-Stoke's equations before or the Newton's second law of motion, these are simply the net forces acting in direction 1 and therefore, these are nothing, but the right hand sides of the Newton's second law of motion.

They can be replaced by the left hand side of the Newton's second law of motion and that is what I will do on the next slide plus all the stresses can be replaced in terms of viscosity multiplied by strain rates.

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Work-Done by Forces-III L4(13/17) Multipliers of u1, u2, u3 in equations 18, 19 and 20 are simply RHS of Momentum equations ( See Lecture 3, slides 13-14-15 ). They are replaced by LHS of Momentum equations. Hence, Equations 18, 19, 20 =  $\rho_{\rm ff} \left[ u_1 \frac{Du_1}{Dt} + u_2 \frac{Du_2}{Dt} + u_3 \frac{Du_3}{Dt} \right]$ Du<sub>3</sub>  $= \rho_m \frac{D}{Dt} \left(\frac{V^2}{2}\right)$ (23)

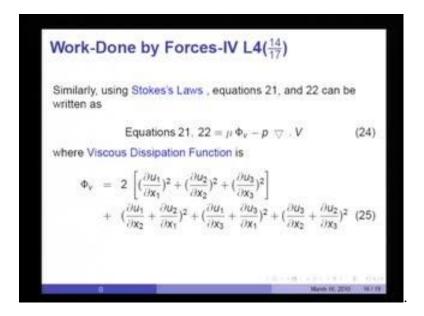
Let us do this first. So, multipliers of u 1, u 2, and u 3 in equations 18, 19 are simply right hand sides of momentum equations, if you recall that on lectures 3 slides 13-14-15.

We have replaced them by left hand side of momentum equations. Left hand side was u 1 D u 1 by D t into rho m u 2 D u 2 by D t and u 3 D u 3 by D t.

This would simply be D u 1 square by 2 D t, D u 2 square by D t and D u 3 square by D t which we write as D V square by 2 D by D t into rho m. (Refer Slide Time: 22:30) These are the first 3 terms that we have expressed; now we look at the remaining terms.

If I replace sigma 1 by minus p plus tau 1 1, sigma 2 as minus p plus sigma plus tau 2 2 and sigma 3 as minus p plus tau 3 3 and tau 1 2 as mu times D u 1 by D x 2 into D u 2 by D x 2 and so on and so forth.

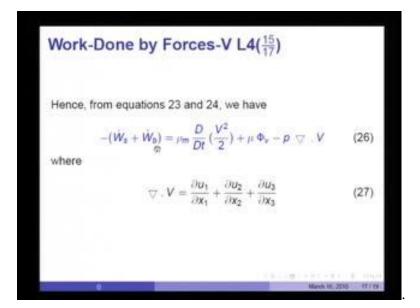
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You will see that the term would be equations 21 and 22 would be simply mu phi v minus p del dot V where phi v is called the Viscous Dissipation Function.

It would take the form 2 times d u 1 by d x 1 square which arises from tau 1 1, d u 2 by d x 2 square, d u 3 by d x 3 square and so on and so forth and del dot V as we recall is simply, d u 1 by d x 1 plus d u 2 by d x 2 plus d u 3 by d x 3.

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Therefore, the total work done terms are simply rho m into D by D t V square by 2 plus mu phi v minus p del dot V. You will notice that phi v will always be positive because it is a sum of all the gradient square.

So, that sum would always be positive and in general and its purpose is to increase the energy level of the mixture. (Refer Slide Time: 24:08) This is the kinetic energy term and this is the minus p d V term or sometimes also called the pressure work term. Del dot v as you know is this.

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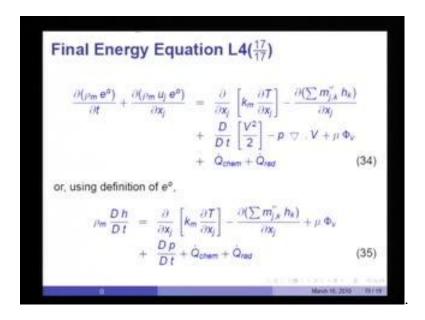
Summary L4(16)	
$\dot{E} = \dot{Q}_{conv} + \dot{Q}_{cond} + \dot{Q}_{gen} - \dot{W}_s - \dot{W}_s$	(28)
where	
$\dot{\boldsymbol{E}} = \frac{\partial(\rho_m  \boldsymbol{e}^{\boldsymbol{\sigma}})}{\partial t}$	(29)
$\dot{Q}_{conv} = -\frac{\partial(\rho_m u_j e^{\sigma})}{\partial x_j} - \frac{\partial(\sum m_{j,k}^r h)}{\partial x_j}$	(30)
$\hat{Q}_{cond} = \frac{\partial}{\partial X_j} \left[ k_m \frac{\partial T}{\partial X_j} \right]$	(31)
Q <sub>pen</sub> = Q <sub>chem</sub> + Q <sub>rad</sub>	(32)
$-(\dot{W}_{a}+\dot{W}_{b}) = \rho_{m}\frac{D}{Dt}\left(\frac{V^{2}}{2}\right) + \mu\Phi_{e} - p \nabla$	V (33)
	PUD 10, 2010 MILLY

By way of summary: we wrote expression for E dot as d rho m e naught by d t; expression for convection was written as minus d rho m u j e naught by d x j minus diffusion heat transfer d by d x j of sum of m dot j k h k.

Q dot conduction was written in this fashion; Q gen was Q dot chem plus Q dot rad and lastly we saw this term is this kinetic energy term, viscous dissipation term and so on and so forth.

You will see that mu phi v is positive and therefore, it tends to increase the rate of energy with time, conduction and if I were to replace Q dot rad as k rad d T d x j and then it would simply get added to that term. (Refer Slide Time: 25:17) This is the p del dot V; this can be both positive and negative and so can this be positive and negative.

#### (Refer Slide Time: 25:22)



The final energy equation then reads as follows. What I have done is simply transported this negative term to the left hand side so that it becomes positive and we have d rho m e naught by d t plus d rho m u j e naught by d x j equal to net conduction heat transfer.

Net conduction heat transfer due to mass diffusion, net kinetic energy generation minus p del dot V plus Viscous Dissipation, chemical energy generation and radiation generation.

Now, if I replace e naught as h m minus p by rho m plus v square by 2 then this term would become simply rho m D h by D t.

The kinetic energy term on the left hand side would cancel with this kinetic energy term and the differential of rho m u j p by rho m which is essentially u j p would simply give me D p by d would cancel partly with minus p del dot V and I will have a term called D p by D t plus Q dot chem rad and so, this is called the Energy Equation written in enthalpy form.

(Refer Slide Time: 26:56) This is the energy equation written in internal energy form. It is this equation which is largely used in flows with or without chemical reaction.

Notice that all it says is that rate of change of enthalpy is equal to the net conduction heat transfer, net mass diffusion heat transfer and total viscous dissipation.

D p by D t - this term is first of all the D p by D t will be partial D p by partial D t which would be of importance in unsteady flows such as one in which explosions are studied plus u into D p by u 1 into D p by d x 1, u 2 into D p by d x 2 plus u 3 into D p by d x 3 these terms are important particularly when shocks are present where very large pressure gradients occur in a given direction, but in low speed force really this term is relatively unimportant and we usually tend to ignore it.

Q dot chem would arise out of the combustion model that one I specified and radiation is to be included in very high temperature reacting flows.

I will conclude here our equations of energy. (Refer Slide Time: 28:35) I would leave you with the simply recall of the mass transfer equation that we derived that was this d rho m omega k by d t and so on and so forth. This is the mass transport equation and then the last one is the energy transport equation. It is these equations that we shall develop further.