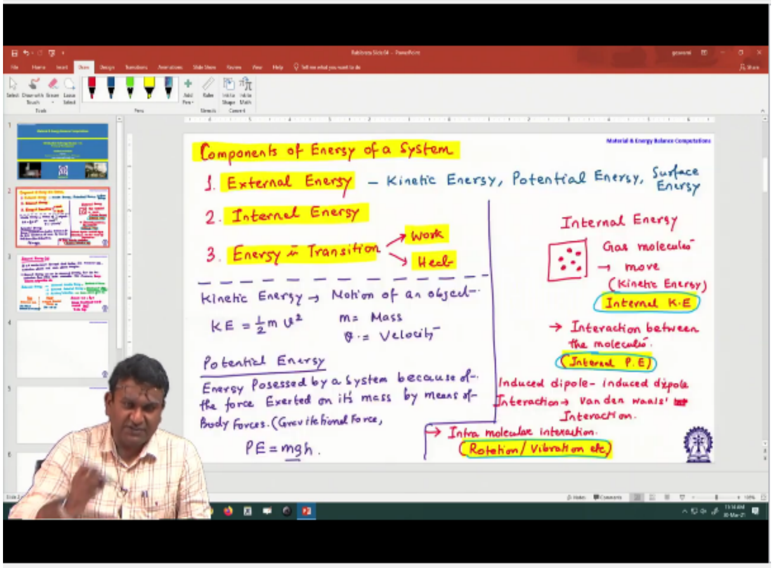
Material and Energy Balance Computations
Prof. Rabibrata Mukherjee
Department of Chemical Engineering
Indian Institute of Technology-Kharagpur

Lecture-41
Introduction to Energy Balance-XI

Welcome back and we will continue our discussion on introduction to energy balance. And, today we are probably going to learn the most important thing. Essentially now, we are all set to essentially learn what is the energy balance or the first law of thermodynamics.

(Refer Slide Time: 00:37)



Material & Energy Balance Computations

Components of Energy of a System

1. External Energy – Kinetic Energy, Potential Energy, Surface Energy
2. Internal Energy
3. Energy in Transition → Work, → Heat

Kinetic Energy → Motion of an object.

$KE = \frac{1}{2} m v^2$ m = Mass, v = Velocity

Potential Energy

Energy Posessed by a system because of the force Exerted on it's mass by means of Body Forces. (Gravitational Force,

$PE = mgh$.

Internal Energy

Gas molecules → move (Kinetic Energy) Internal K.E

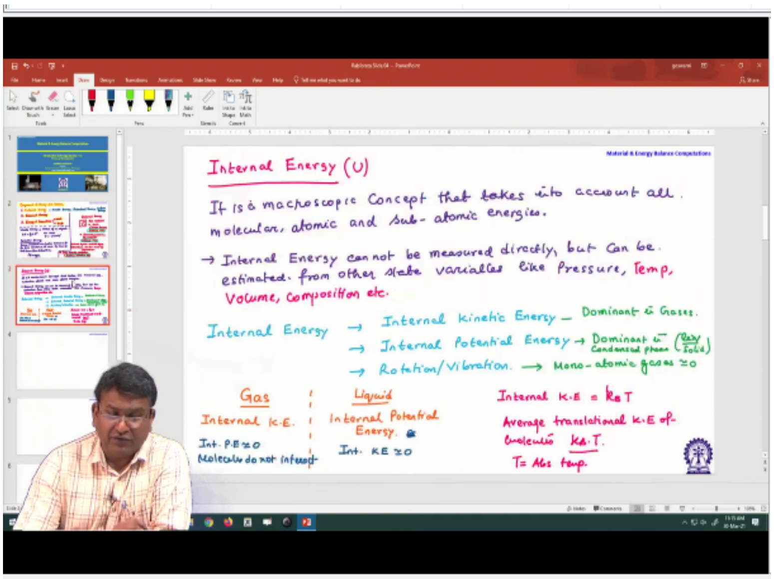
→ Interaction between the molecules. (Internal P.E)

Induced dipole- induced dipole Interaction → Van den waals' Interaction.

→ Intra molecular interaction. (Rotation/ Vibration etc)

But now we are backed up with a reasonably good concepts of different forms of energy of a body, which are the external energy components as a kinetic energy, potential energy and surface energy. The internal energy components and we also now understand about internal kinetic energy, internal potential energy and intramolecular energy that arise out of rotation and vibration. And we also understand about energy in transition that is work and heat.

(Refer Slide Time: 01:09)


Material & Energy Balance Computations

Internal Energy (U)

It is a macroscopic Concept that takes into account all molecular, atomic and sub-atomic energies.

→ Internal Energy can not be measured directly, but can be estimated from other state variables like Pressure, Temp, Volume, composition etc.

Internal Energy → Internal kinetic Energy – Dominant in Gases.
→ Internal Potential Energy → Dominant in Condensed phase (Liquid / Solid)
→ Rotation/Vibration. → Mono-atomic gases ≃ 0

Gas
Internal K.E.
Int. P.E ≃ 0
Molecules do not interact

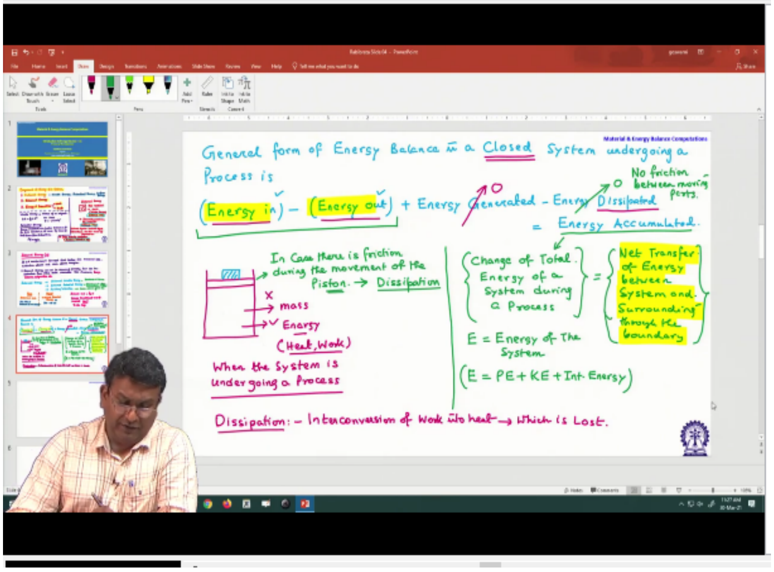
Liquid
Internal Potential Energy.
Int. KE ≃ 0

Internal K.E = $k_B T$
Average translational K.E of molecules $k_B.T$.
T = Abs temp.

So, we have also talked in detail about the internal energy of the components of different type of material and certain interesting things we now understand like a gas, internal potential energy is almost 0 and everything the internal energy is almost dominated by internal kinetic energy. In contrast, in a liquid or a solid internal potential energy is what dominates what forms the major part of the internal energy.

Internal kinetic energy is zero, almost 0, because the molecules do not move, they do not have any relative motion with respect to each other. So, with that I think we are now in a position to again in very simple terms write down the basic form of energy balance.

(Refer Slide Time: 01:57)


Material & Energy Balance Computations

General form of Energy Balance in a Closed System undergoing a Process is

(Energy in) – (Energy out) + Energy Generated – Energy Dissipated = Energy Accumulated.

0 No friction between moving parts.

In Case there is friction during the movement of the Piston. → Dissipation

× mass
✓ Energy (Heat, Work)

When the system is undergoing a Process

{Change of Total Energy of a System during a Process} = {Net Transfer of Energy between System and Surrounding through the boundary}

E = Energy of The System

(E = PE + KE + Int. Energy)

Dissipation :– Interconversion of Work into heat → Which is Lost.

So, general form of energy balance in a closed system undergoing a process is (energy in)- (energy out) + (energy generated)- (energy dissipated) = (energy accumulated). So, this is the generalized form; there are certain things we as usual need to note down. Firstly, we are writing it for a closed system. There is no point in writing the energy balance for an isolated system because that system has certain amount of energy and since no transfer of mass or energy from outside is possible.

Therefore, that energy ideally remains constant. Yes you can do a energy balance for an open system but it comes with certain modifications, which we will take up. So, the most common form of the energy balance you typically write is for a closed system, and we all understand what is a closed system. It is something that will not allow transfer of mass and it will allow transfer of energy.

So, please do understand the transfer of energy can be either in the form of heat or work. When and when does this transfer take place? When the system is undergoing a process. Now, if you say that I have kept a heated block in the surrounding, in ambient condition and there is continuous transfer of energy. Please do understand the system is undergoing a process.

Because the system is not at equilibrium and as we have repeatedly told you can define the state of a system only when it is in equilibrium. So, you now understand what can be energy in like you heat from outside or you do some work on the system. energy out, heat gets transferred from inside or the system does some work. So, this system can also come with a flexible boundary for example.

So, it can come with a piston etcetera, so energy in, energy out we understand. There is one term which you should ask me why at all I have written, because I have essentially written the generalized form and we are talking about systems which do not include nuclear reaction and therefore, this term is always 0. Energy cannot be generated; only in a nuclear reaction or mass defect can be converted into energy.

But in our context since we are not talking about a nuclear reaction therefore energy generated is always 0. Now, one thing I thought initially that I will not touch upon but then I decided for the sake of completeness I will talk. So, the question is what is this particular term dissipation? This is something I will not go into the detail but it may not be a bad idea to give you some glimpse of what is dissipation.

Please do remember dissipation is not heat transfer, transfer of heat. So, what exactly is dissipation? Dissipation is essentially inter conversion of work into heat. And, this heat is lost. We never bother about dissipation; there is a reason for that which I will tell. Now, what exactly is an example of dissipation? A very interesting example of dissipation is what you do in winter mornings?

So, in winter mornings when you get up and let us say you have to attend 8 o'clock morning class, so and you come out of your hotel or your home or your comfort of your blanket, the first thing you do is to rub your hands, you all do that, we all do that and as you rub your hand what you feel is that your palms are getting warm and you feel comfort. So, what exactly are you doing?

By means of this action you are essentially doing some work, you are spending some part of your metabolic energy which you are doing some work and because of the friction that work is getting converted into heat. This is what is dissipation. So, this dissipative heat is actually lost. So, if you talk about a closed system and if there is heat dissipation you must account for that.

Now, in a closed system or in a system which has a moving boundary where can there be dissipation? The dissipation can come in a simple piston cylinder arrangement is if there is in case there is friction during the movement of the piston. Then this will lead to dissipation that is the reason why in all your textbook problems you are always written you are always mentioned a frictionless piston. The moment thus everything happens are is there for a reason.

It is not that we are all used to seeing it frictionless piston and you sort of take it for granted but there is a scientific reason for that. If the word ‘frictionless piston’ is not mentioned as a scientist who has knowledge about all the possible processes that can happen you should always worry you can say that the problem is actually incompletely defined because the extent or the percentage of dissipation is not known.

Therefore, to make life easier for all of us at your level so that you can solve problems and get some answers and write down in your answer scripts. These problems are simplified like there is no dissipation, there is no friction. Interesting thing to note is, so we know that ah when the piston goes upward the system is doing work on the surrounding, it is a negative work.

When the piston is coming down the surrounding is doing work on the system. In case there is friction between the piston and the cylinder; in both the cases, irrespective of whether you have negative work or positive work or in other words whether the system does work on the surrounding or the surrounding does work on the system dissipation is going to lead to generation of some heat and that energy is going to be lost.

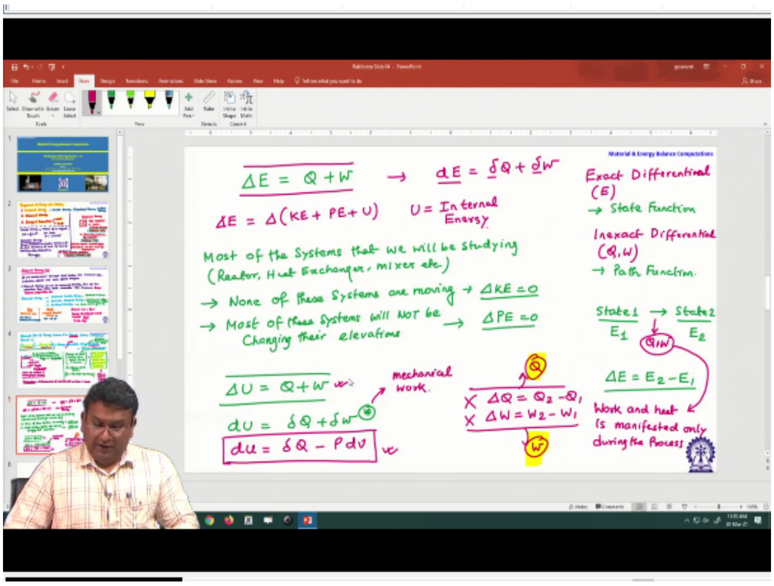
So, irrespective of its not that that when the system is doing work heat you are recovering heat or generating heat it is not like that. Irrespective of whatever is the direction of the process, in case there is dissipation it is always going to loss in heat, work is getting irreversibly converted into heat and which is getting lost. For simplicity, in this course beyond this point we will not talk about dissipation. So, that is all about it.

So, we set under the framework of this course or the assumption that there is no friction between the moving parts, dissipation can be neglected. So, this essentially takes us to a form that upon simplification one can write
(change of total energy of a system during a process) = (net transfer of energy between system and surrounding through the boundary).

So, change in the total energy of a system during the process so that is the energy accumulation term. And, {(energy in) – (energy out)} is essentially the net transfer of energy between the system and surrounding through the boundary. So, this is you can say is sort of the functional form, it still a sort of a understanding, you can understand the energy balance through in this way.

So, what is the total change of energy of a system? Let us say, Energy of the system, E = PE + KE + internal energy. comprises of potential energy plus kinetic energy plus internal energy. This we all know, so the sign of internal energy of course you can also add surface energy does not matter. the sign of internal energy is u.

(Refer Slide Time: 13:35)



Material & Energy Balance Computations

$\Delta E = Q + W \rightarrow dE = \delta Q + \delta W$

$\Delta E = \Delta(KE + PE + U)$ $U =$ Internal Energy

Most of the Systems that we will be studying (Reactor, Heat Exchanger, mixer etc.)

→ None of these Systems are moving → $\Delta KE = 0$

→ Most of these Systems will NOT be Changing their elevations → $\Delta PE = 0$

$\Delta U = Q + W$

$dU = \delta Q + \delta W$ → mechanical work.

$\boxed{dU = \delta Q - PdV}$

$\times$ $\Delta Q = Q_2 - Q_1$

$\times$ $\Delta W = W_2 - W_1$

Exact Differential (E)

→ State Function

Inexact Differential (Q, W)

→ Path Function.

State 1 → State 2

E_1 Q, W E_2

$\Delta E = E_2 - E_1$

Work and heat is manifested only during the Process

So, we can write the this above equation in the form of

$\Delta E = Q + W$ where this transfer of heat is taking place either by heat transfer or by work done. I prefer to write as Q plus W you can write Q - W also; different books follow different notifications or that is not a very important thing. Now what you need to understand that this ΔE or in the differential form you can write dE equal to δQ plus δW, you must all understand the difference between ‘d’ and ‘δ’ is energy (E) is an exact differential, a state function and work (W) and heat (Q) are inexact differentials, path functions.

And this is related to this being a state function and this being a path function. Or, even to understand it in one step. So, when the system undergoes a transition from state 1 to state 2, there is some energy of the system at state 1, there is some energy of the system at state 2, therefore you can always write, $\Delta E = E_2 - E_1$; but no work or heat is associated with state 1 or state 2 and work and heat is manifested only during the process.

So, we have discussed it many times but I prefer to discuss it again. only during the process and so you cannot write a term like ΔQ or you cannot write a term like ΔW; both of them are wrong. You can only have Q or W that is released or performed during the process. I hope this discussion should be clear to all of you. because many people have a little bit of fussy concepts between this exact differential, inexact differential.

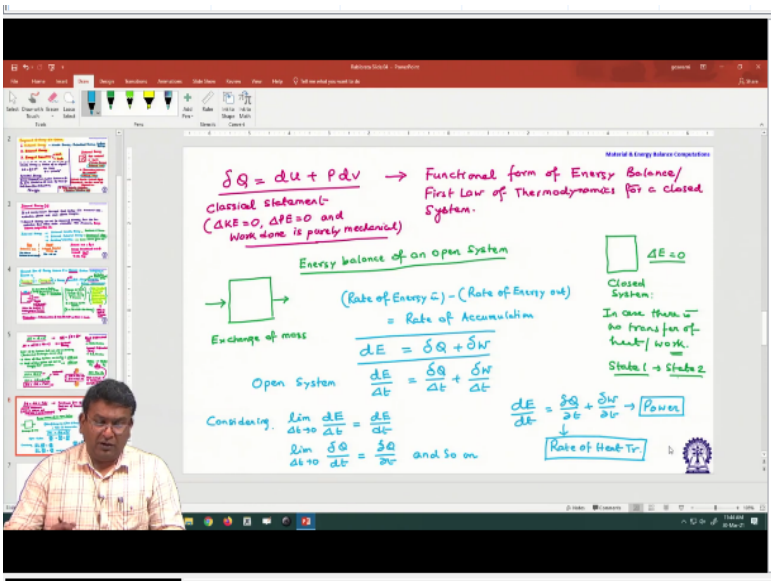
So, anywhere you write something like ΔQ or dQ, it is completely wrong. and it is wrong because if you have let us say d of some variable then you integrate it between its initial value and final value. Let us say, you are integrating dx between x 1 and x 2, so you get x 2 - x 1. So, x 2 must be defined, x 1 must be defined. Please do understand the value of work for the initial state is not defined.

Value of work for initial final state is not defined. So, you cannot write $W_2 - W_1$. So, coming back to our discussion over here; so this ΔE is actually the change in the kinetic energy plus potential energy plus internal energy, where U is the symbol for internal energy. Now, for most of the systems that we will be studying like a reactor, heat exchanger, mixer or whatever separation units like distillation column.

Everywhere there is an energy balance, but none of these systems are moving or most of the systems that we are studying are stationary systems. So, if they are not moving then what we have delta KE = 0. Also most of the system or almost all of the system will not be changing their elevations. So, that would mean delta PE is equal to zero. So, what we are essentially left with for most of this thermodynamic system of typical closed systems that we will be investigating we actually have $\Delta U = Q + W$.

Or in the differential form it is, $dU = \delta Q + \delta W$; and, if we primarily consider this to be the mechanical work then we are left with an expression, $du = \delta Q - Pdv$ as we know $\delta W = - pdv$ for mechanical work. So, this is a very, very important expression that we might be requiring in future. either of them is fine but this is something that is quite frequently used.

(Refer Slide Time: 20:48)



Material & Energy Balance Computations

$\delta Q = du + Pdv$ → Functional form of Energy Balance/ First Law of Thermodynamics for a closed System.

Classical statement (ΔKE = 0, ΔPE = 0 and Work done is purely mechanical)

Energy balance of an open system

Exchange of mass

(Rate of Energy in) − (Rate of Energy out) = Rate of Accumulation

$$dE = \delta Q + \delta W$$

Open System

$$\frac{dE}{\Delta t} = \frac{\delta Q}{\Delta t} + \frac{\delta W}{\Delta t}$$

Considering $\lim_{\Delta t \to 0} \frac{dE}{\Delta t} = \frac{dE}{dt}$

$\lim_{\Delta t \to 0} \frac{\delta Q}{dt} = \frac{\delta Q}{\partial t}$ and so on

ΔE = 0

Closed System:

In case there is no transfer of heat/ work.

State 1 → State 2

$$\frac{dE}{dt} = \underset{\boxed{\text{Rate of Heat Tr.}}}{\underset{\downarrow}{\frac{\delta Q}{\partial t}}} + \frac{\delta W}{\partial t} \rightarrow \boxed{\text{Power}}$$

Or, one can essentially write that δQ = du +Pdv. This is the functional form of first law of thermodynamics. This is a very powerful equation for a closed system. However, there can be some situations so you can, this is you can say the classical statement of the first law, of course for simplification that ΔKE = 0; ΔPE =0; and the work done is purely mechanical. But there can be systems. So, this is for a closed system.

We may have to do energy balance for open systems also. There are systems which are open system and there is the energy balance plays a key important role. So, we sometime find it desirable to use the first law as a rate equation that expresses the instantaneous or the average rate at which energy enters a control volume or a control surface as heat work and rate at which the control mass changes.

So, it means essentially that so now if you let us not get into the classical definition. Let's talk about the energy balance of an open system, so in comparison to a closed system for a closed system if it is not undergoing any process the change of energy will be zero. That is in case there is no transfer of heat or work, ΔE = 0 and when we were defining this closed system we talked about when ΔE = 0 the system was undergoing a transition from state '1' to state '2'.

The only consideration we had was state 1 was at thermodynamic equilibrium and then it moves on to state 2 which is also a thermodynamic equilibrium. We did not bother about the time. Because in classical thermodynamics time is never defined between or what is important is that the systems must be in equilibrium. But what happens in open system? So, in open system there can be exchange of mass along with exchange of energy.

So, there can be heat transfer and in addition to that exchange of mass means that when some mass is coming into the system not only the mass of the system is increasing but the energy of the system is also increasing because the incoming mass is bringing in some additional internal energy. And similarly when mass is leaving that is also taking away some internal energy.

Now if you have a continuous process what you need to bother about the rate of exchange of this energy with time. So, we are essentially drifting a little bit from the realms of classical thermodynamics where we are essentially looking at the rate at which energy is entering and energy is leaving. So, the classical statement essentially changes a little bit,
(Rate of energy in) – (Rate of energy out) = (Rate of energy accumulated)

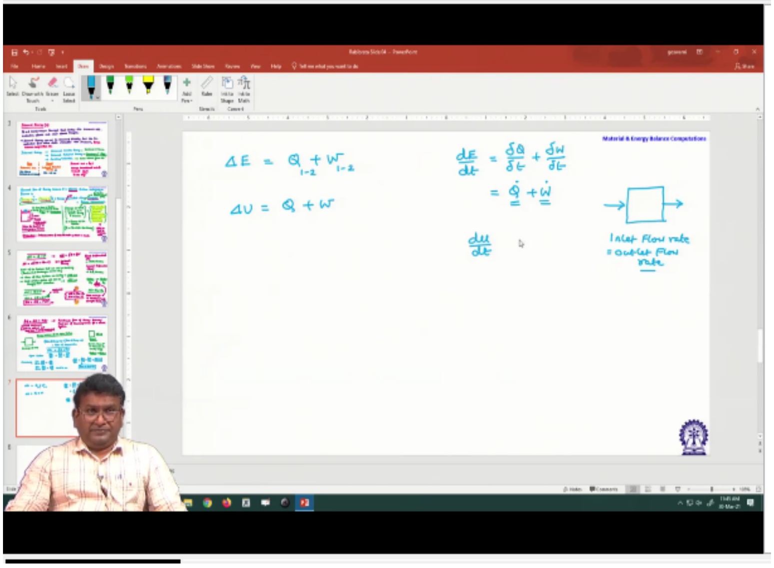
So, for a open system essentially so we are neglecting the energy generated and energy dissipated term. So, for a open system what happens is aa the form of the equation changes to rate of energy in minus rate of energy out equal to rate of accumulation. Or, essentially we are now looking at not exactly in terms of $dE = \delta Q + \delta W$ which is modified for an open system as, $dE/\Delta t = \delta Q/\Delta t + \delta W/\Delta t$. And, considering for a limit of $\Delta t \to 0$, we get
limit $\Delta t \to 0$ $dE/\Delta t = dE/dt$; limit $\Delta t \to 0$ $\delta Q/dt = \delta Q/\partial t$ and so on. And, $\delta Q/\partial t$ and $\delta W/\partial t$ are essentially the rate of heat transfer and rate of work done which is nothing but power respectively. And, the final form of the equation is, $dE/dt = \delta Q/\partial t + \delta W/\partial t$.

So, I will just summarize what we talked about. We essentially talked about the energy balance in an open system. And, in an open system what happens is so in open system how much energy is entering? how much energy is entering is actually a function. So, if you allow the time window to be 1 minute let us say 500 joule energy is entering. But if you allow the time window to be 10 minute then ah 5000 joule is entering.

Therefore, the total amount of energy that is entering does not have any sense for a open system, what you need to bother is the rate at which energy is entering and the rate at which energy is generated. So, essentially we drift from the classical understanding of thermodynamics in converting the first law into a rate form which can be used for an open system.

And we are assuming that delta t is equal to very small therefore despite this mass and energy entering and leaving the system never deviates from equilibrium. So, that is an assumption we have talked about an infinitesimal process. So, in doing so we are drifting from strictly classical viewpoint of thermodynamics as classical thermodynamics deals with system that are at equilibrium and therefore it is time independent but here essentially we are looking at the rate form.

(Refer Slide Time: 30:00)



Material & Energy Balance Computations

$$\Delta E = Q_{1-2} + W_{1-2}$$

$$\Delta U = Q + W$$

$$\frac{dE}{dt} = \frac{\delta Q}{\delta t} + \frac{\delta W}{\delta t}$$

$$= \underline{\underline{\dot{Q}}} + \underline{\underline{\dot{W}}}$$

$$\frac{du}{dt}$$

Inlet Flow rate = outlet Flow rate

So, we can summarize by saying that we can write the energy balance as dE = Q + W one can write state 1 to state 2, this is for a closed system and one can write this to be,

$\Delta E = Q_{1-2} + W_{1-2}$ for closed system and $dE/dt = \delta Q/\partial t + \delta W/\partial t$ for open system.

Q dot and w dot are power and rate of heat transfer under the simplification that we are essentially looking at static systems which do not there is no change in potential energy and kinetic energy etcetera.

So, we can write this to be equal to dQ = Q + W. Same thing over here, so if you now have a flow system where the inlet flow rate and outlet flow rate are same, then we again have a system where there is no change in the kinetic energy and eventually we will actually be looking at how the internal energy changes with time so with that we are running out of time and probably we will stop our discussion over here for the time being.