Indian Institute of Technology Madras

NPTEL

National Programme on Technology Enhanced Learning

COMBUSTION

Lecture 12
Combining Chemical and Thermal Processes 2

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So we have been moving on to trying to do something with the chemical kinetics data that we have been used to so far by trying to combine it with the thermal information that it goes with the means there is a heat transfer that is associated with the chemical reactions that we need to worry about and so can we put them together it is possible to put them together in some simple frameworks because we do not want to get involved in the flow processes and the mixing processes.

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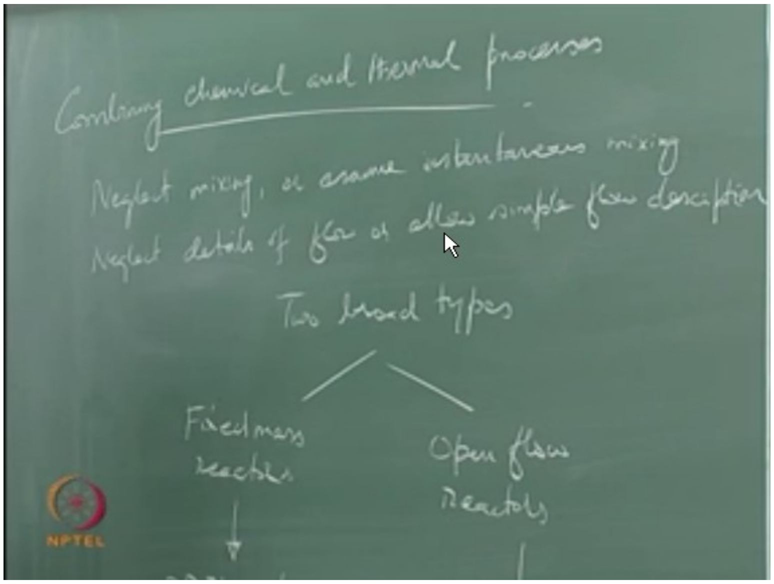

Combining chemical and thermal processes

Neglect mixing, or assume instantaneous mixing

Neglect details of flow or allow simple flow description

Two broad types

Fixed mass reactors

Open flow reactors

So the first thing that we will try to assume is, is it possible for us to actually neglect mixing and typically evenly but what do you mean by saying neglect mixing is that may be mixing is not there it is not important it is not it a significant extent or it is there a whole lot and almost lot of things are actually getting instantaneously mixed which is actually closer to truth okay in reality if you are trying to adopt these kinds of models simplified models where we are only interested in combining chemical and thermal processes without bothering about flow and mixing.

Then typically you are looking at situations where the mixing is almost instantaneous right so you do not have to worry about it okay we will try to qualify this as when we are exactly neglecting versus when it is exactly instantaneous as we go along particularly for the plug flow reactor where we now could be looking at a simple flow description for the plug flow but for most other parts we should not have to worry about the flow because it is too complicated.

Let us not worry about it either right so it is not as if like you do not really have a flow but when, when there is a flow it is too complicated for us to worry about may be baby it is not important for us to worry about that level of complication is it possible for us to deal without having to take it account flow description as much as we can and also by neglecting mixing if you try to adopt this kind of a framework you are disregarding flow and mixing then we have roughly broadly two kinds of approaches one is what is called as fixed mass systems or open flow systems.

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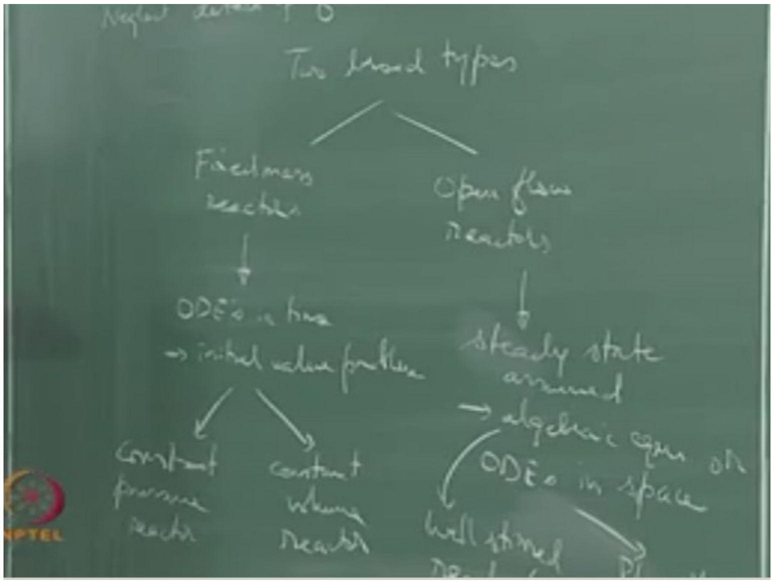

So the fixed mast reactors our goal list we now have a fixed mass of material what started out to be reactants in the, the beginning for the same mass of the reactants the reactants now proceed to become products right so in a chemical reaction the mass has not changed so it is the same mass that we are talking about but originally we started out having reactants and later on you are now having products when we first started adopting chemical thermodynamics dynamics right.

When we are looking at the equilibrium thermodynamics of the chemical reactions we started by talking about initial reactants and final products but whenever really worried about the time evolution between the two okay for all we cared it is could have taken ages in reality combustion reactions take, take a jiffy there does not take a lot of time okay but whatever it is we would like to see how this evolution happens between initial reactants to final products through maybe intermediates right.

If you are able to take into account the detail chemistry as much detail as we would like to do right so this is what we are trying to do now as opposed to what we were trying to do earlier on with our equilibrium thermodynamics approach okay so in this sense this is not an equilibrium situation at all we are looking at a set of reactants that might be in equilibrium initially but you now look at departure from equilibrium as the reaction commences and, and, then we now get into a situation value to finally get products which could be in equilibrium ultimately right previously we looked at only these two n states but now we are looking through these states so this is obviously going to be a problem that describes our changes as an evolution in tummy for we need to have a time description of it.

What we will actually be looking for is ordinary differential equations in time for typically temperature and concentrations of, of all the species okay see these are the two things that we should be looking for on the other hand in the open flow reactors we could afford to make an assumption of steady state whichever church which is more convenient for us we don't have to worry about evolution in time and that, that means everything that is happening, is happening at all times okay.

So if you now try to do that than your time derivatives in Euro des will go away and if you had 0 des in time and you had to get rid of the derivatives you now are stuck with only algebraic equations you see and that is actually like a direct consequence of applying this kind of formulation without the time derivatives you now get rid get, get to algebraic equations which, which is which is the model called the well stirred reactor and but, but you could still also do some more things like maybe you say well.

I know how to solve goodies okay I have done this here we are not going to solve though these but let us suppose that we formulate the problem in the OU des and we suppose that we can solve the OU des Valerie Kay if we could solve o de x in time work and I saw would ease in space so if you have to solve Woody’s in space is ordinary differential equation in space that means I can allow for only one special variable right that simply means that I can now begin to account for one dimensional variation in, in space okay.

So I could adopt like a one dimensional approach which will lead to the plug flow reactor so you will now have Woody’s in space so you will now have a d by DX kind of derivatives showing up over here in this so to picture eyes what we are talking about in the kinder case of the fixed mass reactors you could do this as a either of a constant pressure reactor or a constant volume reactor ideally this is this idealization as you can see this is all these are idealizations right so or these are idealizations that are effective the simplifications so in a simplified system we now think about like a constant pressure fixed mass reactor.

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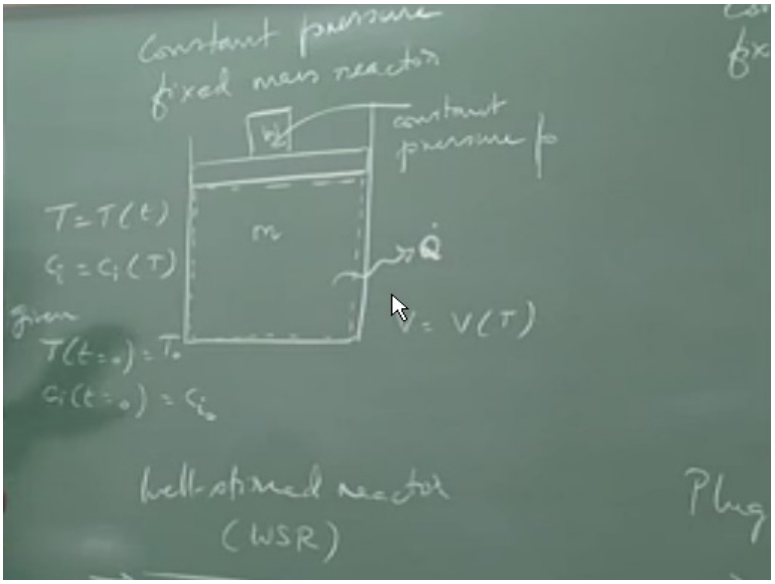

So you can think about a template geometry which is like a piston cylinder arrangement where the piston has a constant weight in a recall especially in varying gravitational field so we have to say that there for maybe now say that this is going to be exerting a constant pressure the pressure is constant but the volume can change so as the temperature changes with whatever heat that you are going to try to remove out of the chemical reactions.

The volume can change so this is this is volume as a function of time there so here our interest as I said is we are now trying to write Oh des in temperature and the concentrations of the species so we are looking for time evolution of temperature and time evolution of concentrations of the species okay so if you now started out with certain species like CI not for I going from 1 to capital n and of course we will obviously start with reactants so if you want a number your species as one is equal to the first reactant this 2 is equal to the second reactant and so on12 minutes and so on will have non -zero values.

But if you now have your n, n- 1 and all those things is like products they would typically have 0values right and typically you know even intermediates will have to start with you will have 0 okay so you will have non-zero values for reactants and zeros for intermediates and products due to do start wit for CI 0 and he also can indicate an initial temperature for this and then you now have the clock ticking greater than 0.

And then now you integrate your oh de system in time to get how this evolution happens as a, as a offshoot of this you could now also try to find out how the volume changes in time alright and we will go through how to do that you have a constant volume fixed mass reactor where you know just to have a box okay you do not even have a piston that could, could move back and forth to maintain the constant pressure so the volume is fixed.

So the pressure obviously is going to change in time so the problem is posed exactly similarly to what we have done before as far as the Eau de set is concerned except we will now see some changes in the equations because you are now keeping the volume fix rather than letting the pressure, pressure fixed and consequently as an offshoot we should be able to also find out how the pressure changes in time so this is how this problem would be post on the other hand.

If you now look at the open flow reactors the first of which is the well stirred reactor it is, it is in a way is you see a counterpart of this that means or you could say you could take the counterpart of either of these as a matter of fact let us not let us not worry about that but there is a lot of flow that is going on inside okay which we do not want to worry about that means we will not worry about the spatial variation of things inside how they are actually spatially distributed okay.

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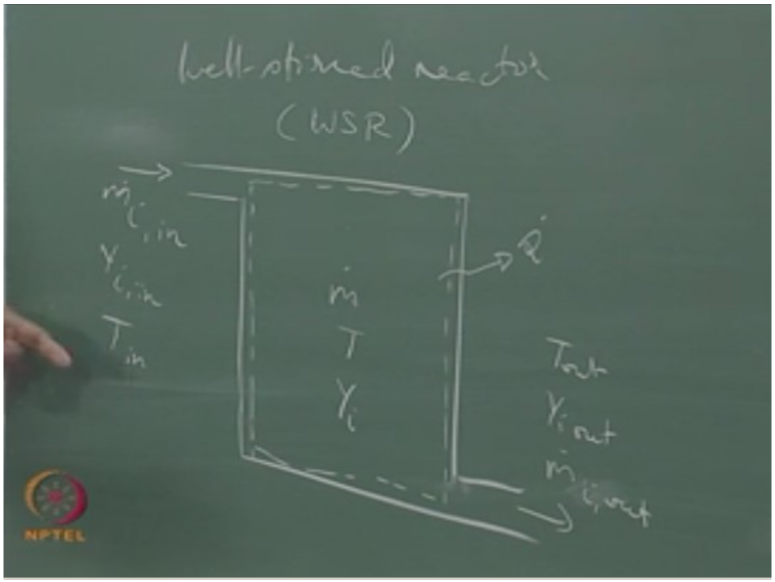

Then we are also making the steady state assumption that means we want to actually look at how the system works under steady state conditions right that means we are not looking at a time variation as well okay so what it simply means is this is a model that is going to tell you if I put in reactants of certain concentrations here at a certain temperature okay with mass fluxes for each of those like this summed over some dough word to get you a certain m dot which is constant okay so the mixture m dot is going to be constant throughout the system right from Inlet to outlet okay.

But the but the but the individual species m dots could change such that the mixture and dot is constant so ∑mi in overall I will be equal to ∑mi out overall I equal to m dot okay that is the way it this is going to work out the question is if I were to put in these reactants in at this particular temperature right what is it that I am going to get out for a given volume of this that is not a bad problem to think about right so if I have a box and then I am going to put in certain reactants it is okay for me to expect what to get out of this box right.

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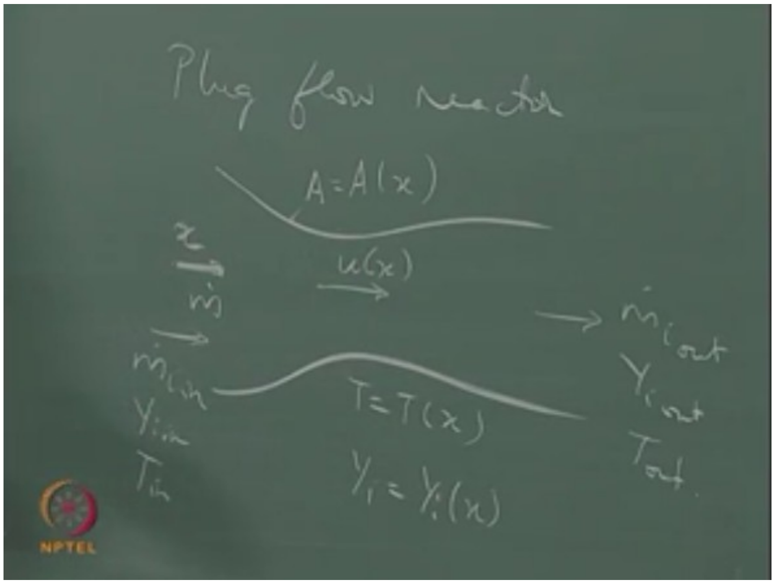

So we will find that this is actually pretty useful yeah and, and, and I will explain to you how useful you useful address in, in different contexts then as I said you can also allow for some simple flow description and the simple flow description is essentially in a one-dimensional sense what we will now allow for is a quasi one dimensional variation k so quasi means that you will allow for like a area variation to happen along the flow direction largely speaking so your a is equal to a of X that is given right.

And you know allow for everything to vary as a function of X the means your temperature concentrations density pressure velocity okay because your area is changing the velocity will change below because the velocity changes the pressure changes the pressure changes so the density changes the density changes the temperature changes everything changes because of this all as a function of X nothing in nothing as a function of time okay.

So we will start with reactants as usual it is a steady state situation so m dot s is the same we measure things along x direction as I as a variation there so this is typically how we are going to deal with these different situations alright so let us, let us now look at how to deal with yeah, yeah which one is similar to that the combustion we use in aircraft we are those take up this question after I finish everything okay the answer is the combustor in an aircraft for example is a is a is a combination of about two or three and PF sorts put together in a network .

Okay or in other words you could model your combustor that way if you do not want to get to actual physical details of how things are distributed and so on we could we could come up with a network in which you now say the primary zone is one WS are the secondary zone is another wsr and the tertiary zone like the dilution zone could be a PSR or a WS are depending upon whether you want the spatial variation or not okay so reality is more complicated than these but these things could now be used as building blocks to create a like a network that would simulate the reality all right.

You could think about this as something that can that can work easily for like a rocket nozzle for example so this is not a bad idea well stirred reactor it many times works well for things like furnaces okay so where you have like a free constant feed and then you have exhaust going out so you could sometimes or many times as a matter of fact Model, Model those kinds of complicated combusted geometries with AWS are look at rockets yes sure it is possible okay.

We will look at why we need to have networks for like a like an aircraft, aircraft combustor because we have a primary zone where you having a stoichiometric combustion first and then you have like a, a, a few lean combustion next and then you now have a tertiary zone which is not too much of reactions and so on so that is the reason why you need to have a network otherwise you could actually have a frou-frou crude approximation.

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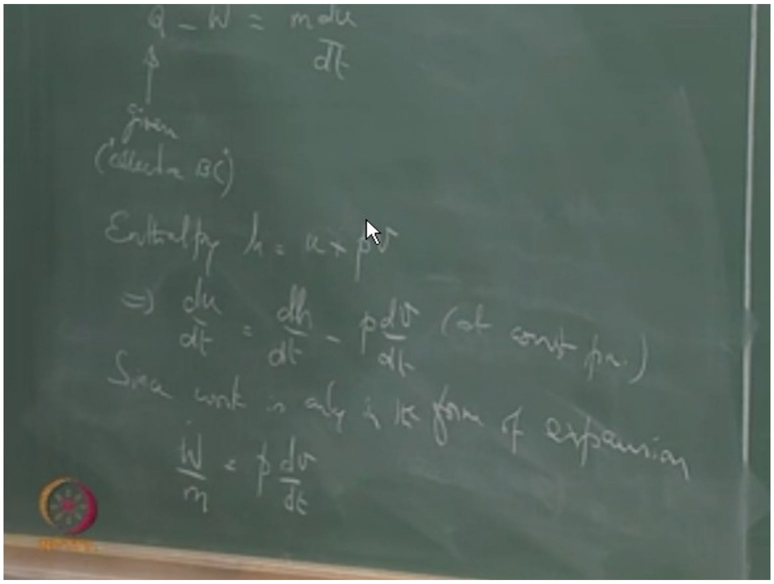

$$Q - W = m\frac{du}{dt}$$

given (also a BC)

Enthalpy $h = u + pv$

$$\Rightarrow \frac{du}{dt} = \frac{dh}{dt} - p\frac{dv}{dt} \text{ (at const pr.)}$$

Since work is only in the form of expansion

$$\frac{\dot{W}}{m} = p\frac{dv}{dt}$$

You could have a combustor replaced by a double wsr that is fine so right so our goal here this is too fine dilution of t CI + v given initial conditions and then that is t not see I not v not so this is what is called as a initial value problem ivp so how would you do this essentially the broad outline for any of these approaches is as follows as far as specie concentration is concerned we have to now apply conservation of mass of individual species okay.

As far as temperature is concerned we have to look at a global energy balance so of course what will happen is you will find that each of these equations depends on all the variables that means equation for the at species mass balance will depend on all concentrations, concentrations of all species see I and T and the global energy balance will not only depend on T but also all the sea ice so you now get a system of equations right so this is what we will do and it is more straightforward for us to think about a global energy balance in terms of the first law of thermodynamics okay.

So you just have to apply the first law of thermodynamics right away so energy balance is first law of thermodynamics that means cumin is the Q dot minus W dot equals MDU DT now this is speed is given right in a sense if you think about it if you were to if you are a partial differential equations expert and you were like raring to go on trying to get multi-dimensional spatial variation as well as temporal variation simultaneously all together right.

You will now say this is a box with these boundaries and then there are like boundary conditions that need to be given I need to tell what should be the heat flux here what should be the heat flux here on this wall what should be the heat flux on this wall and so on separately right but here we decided that we will not worry about any spatial variation right you are looking at only temporal variation so we are looking for Oh des in time and therefore this is like a some sort of like a collective boundary condition.

So it is like what is the net heat, heat flux across all the surfaces okay so this is this is supposed to be like a given you can think of this as a collective you do not require a boundary condition at all here but if you were to have boundary conditions in a real problem how to convert that into a given property here is what you're looking for in this so I would say collective bc within coats now we have to look at what is w dot therefore it is not very difficult for us to fathom I mean w dot is essentially going to be like the expansion work right.

So we let us look at how that comes about so enthalpy oh h equal to u plus PV right now most of the time in fluid mechanics the gas dynamics you wouldn't really worry about what the sketch is okay but we are dealing with a multi-component system that means mixture of species right and then in addition to that we also have chemical reactions going on so we will have to actually distinguish between standard heat of formation and sensible enthalpy for each of those species so this is pretty much now going to actually grow like a genie out of a bottle soon okay anytime you see a very innocuous H in your combustion class be prepared to see that it is going to now just grow like a genie right.

Because it is now going to be taking care of all the species in there and for each of those species you have to look at the standard heat of formation and it is sensible enthalpy so we will we will do that soon okay so, so long as we not we are more innocent at the moment right we could simply write this as G you over DT equal to D H over DT minus P DV over DT p is constant so we do not have to worry about changing its changing with time so this is constant pressure constant pressure now then since, since work is only in the form of expansion right we can easily write that w da divided by M that is the rate of work per unit mass of the system is equal to p times DV over DT right.

So from here you now put, put things together we already have d you over dts equals 2 dot minus W dot divided by M W dot divided by M is already p DV over dt and then we have d you over dt is equal to D H over DT minus P DV over DT so putting, putting everything together this simply means that Q dot divided by M is equal to D H over DT this is something that we already seen earlier okay when did we see this the moment we actually define heat of reaction so when we said heat of reaction is the heat that is released in a chemical reaction which started out at a star at a certain temperature and pressure and came back to the same temperature.

And pressure is what we said ok and at that time we noticed that the heat that is released during this process is the same as the enthalpy change ok there is a reason why to find the adiabatic flame temperature at constant pressure we were requiring enthalpies of the reactants and products that is the initial state to the final state and this, this exactly safe that Q dot is the heat that is released from this system okay and per unit pass H is actually per unit mass.

So the reason why we have to divide by mass here k small His per unit mass I will I will explain this notation pretty soon it is going to get a little bit more complicated as I said right so the chain so Q dot is the one that is making it equal to D H over DT if it were simply queue that means you do not have to worry about the rate of heat that is going out it is a total heat over what about time then you will simply have h okay.

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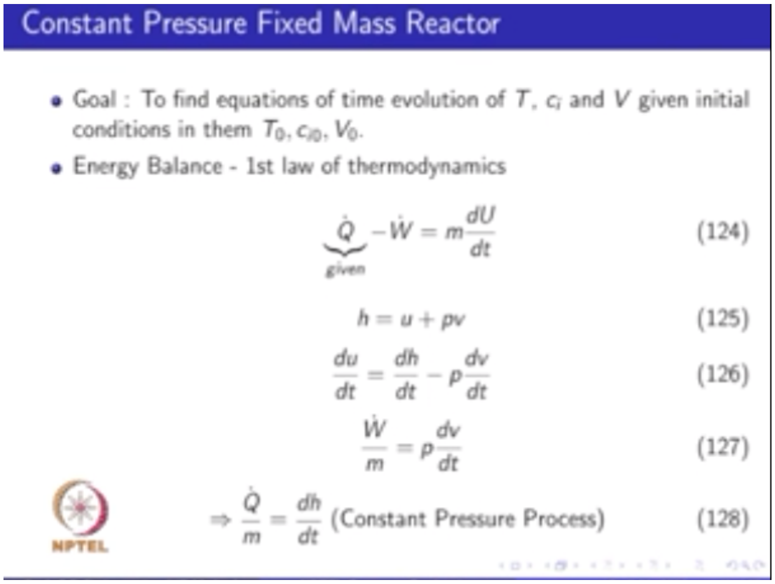

Constant Pressure Fixed Mass Reactor

- Goal : To find equations of time evolution of T, c_i and V given initial conditions in them T_0, c_{i0}, V_0.
- Energy Balance - 1st law of thermodynamics

$$\underbrace{\dot{Q}}_{given} - \dot{W} = m\frac{dU}{dt} \tag{124}$$

$$h = u + pv \tag{125}$$

$$\frac{du}{dt} = \frac{dh}{dt} - p\frac{dv}{dt} \tag{126}$$

$$\frac{\dot{W}}{m} = p\frac{dv}{dt} \tag{127}$$

$$\Rightarrow \frac{\dot{Q}}{m} = \frac{dh}{dt} \text{ (Constant Pressure Process)} \tag{128}$$

So this, this is primarily because it is a constant pressure process the beans in the constant pressure process the specific heat, heat flow rate is equal to the rate of change of enthalpy okay so this, this comes about namely because of constant pressure I will contrast this with what you will get for Q dot x em in the constant volume case intuitively we should expect that this should contribute only to the internal energy change because the pressure work is forbidden in a, in a constant volume situation you do not have a you do not have room to expand right.

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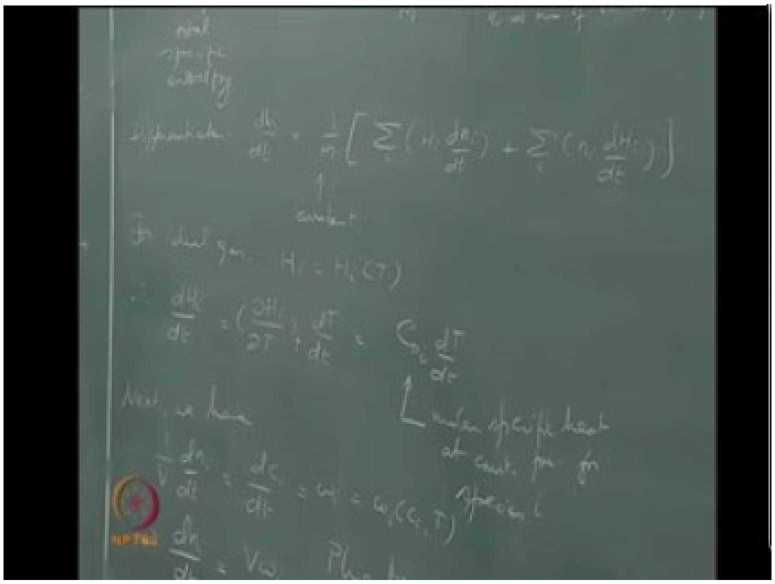

So we will be able to see the contrast in the first law of thermodynamics when you apply this sit to the constant volume case next but at the moment we will stick to the constant pressure case now H is now equal to H over m okay now this is the total specific enthalpy this is the total enthalpy right so it says Pacific that means it is per unit mass okay the next thing I am going to say is something called molar specific okay when I do not say mass specific then it is implicitly per unit mass.

If I have to say per unit mole then I will have to specifically say molar specific okay so the moment this is more specific regardless of how you want to count here enthalpy okay the total enthalpy you want to now say mass times the specific enthalpy will give you the total enthalpy or number of moles times the molar enthalpy will also give it a total enthalpy the total enthalpy is the same right now so you are now going to bring in the molar enthalpy the molar specific enthalpy.

So that is a given by ∑i equals 1 to n ni h I / M where hI is capital H I is the molar specific enthalpy of species I and ni of course is number of moles of species I number I am sorry number of moles species I or I at species whichever way you want to call it now see we use a capital H I for these molar specific enthalpy all right we will not really worried about a total molar specific enthalpy at all then so we do not have to worry about what, what symbol we will use for it okay.

So this is the notation here for what we are doing now you let us say let us suppose we now differentiate this is a different sheet different shape differentiate this obviously with respect to time you are looking at what happens with respect to time so the mass is constant so you can happily take that out the denominator so this is constant that is what fixed mass systems are all about but unfortunately both the total both the number of moles of each species, as well as the molar specific enthalpy of the species are changing in time okay. Why would they change well why would well the number of moles changes because reaction is happening okay.

So you start out with some so many number of moles of reactants they added at the end of the reactant you do not have them, so that means that has changed right and in the process some number of moles of products they did not exist for has been produced and so on so that is obvious. Why would the capital HI change temperature okay, so capital H I the next thing is we are going to write this as the standard heat of formation + the sensible enthalpy.

The sensible enthalpy depends on temperature the temperature is going to change in time as a reaction happens there for the sensible and talk to change is therefore the molar specific enthalpy is going to change, so you have to take in account the change of both with respect to time. So that is σ I am going to I am going to get tired of riding i σ i = 1 to n every time so I am just simply going to say Σ I and then that is a hiDni over + σ i dh_i over dt okay.

For ideal gas a Hi is a function of temperature only and that is the expression that we were talking about, that is it is it has a standard heat of formation and the sensible enthalpy and the sensible enthalpy is the one that is changing with temperature okay, so if you are now looking at the derivative of this with respect to temperature it is a derivative of the sensible enthalpy with respect to temperature at a constant pressure okay.

What is that okay therefore dhi over dt is do a hi over δ t at constant pressure dt over d right, so this is C_{PI} dt where this is now molar specific heat or of species I, molar specific heat at constant pressure for species I, that means if in case you did not think about this every species is going to have its own specific heat this is something that of course we noticed during the equilibrium calculations for adiabatic flame temperature okay.

Just wanted to remind you second thing we are using a capital C for molar specific heat to go with a capital H for the molar specific enthalpy alright, for the for the specific heat right there is per unit mass. So this is this would be joules per mole Kelvin all right that would be the SI units for this the standard one is dose per kg Kelvin we will lose a small c over there okay. So we have that n, next so we are trying to evaluate these terms here.

So next we have 1 over dn_i over dt = dc_i over dt = ω I this is how we define these things if you remember right, so you know run up to looking at the law of mass action this is how things were defined for you alright. So that is that is beginning to look at combining chemical kinetics and thermal information you see so this is coming from your kinetic c ω i is actually a function of C_I , T you have that huge expression you see you remember right, that is like σ i = 1 to capital M for the number of reactions μI k double prime - μ ik single Prime and blah some huge expression.

Which had all the Ci is thrown in there and the temperature in the arena is expressions for each of those reactions right that is an ugly looking expression there we are spared of that because I am not going to write this out but it is there with you notes okay. Now therefore di dt is = to V ω I alright, so for these the plug these above bow is here we can now say dh over dt is =to Q . / M we can plug that for the dh over dt and for dni over dt_I am going to plug V ω I and for cap d capital HI over dt I am going to plug CP_I dt over dt right.

That is all I am going to do does not look like a big problem or the M gets cancelled you have a Q. Over M you have a 1 over M so the M gets cancelled.

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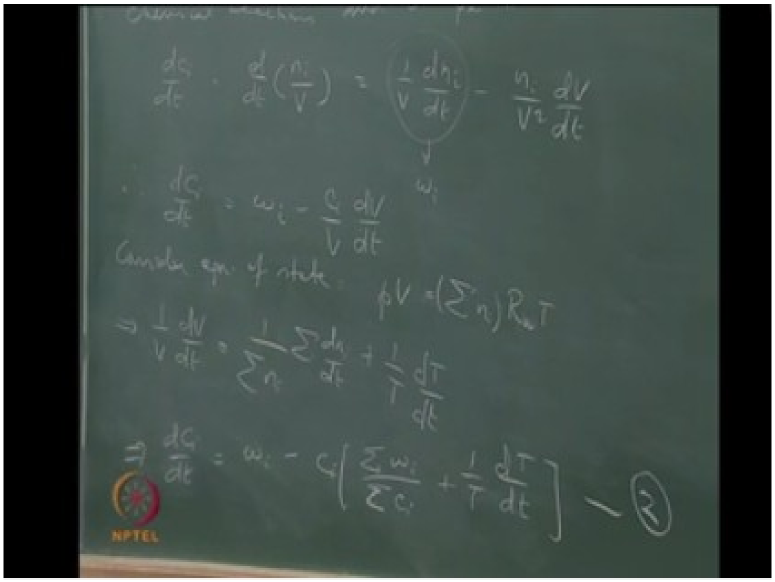

$$\frac{dc_i}{dt} = \frac{d}{dt}\left(\frac{n_i}{V}\right) = \underbrace{\frac{1}{V}\frac{dn_i}{dt}}_{\omega_i} - \frac{n_i}{V^2}\frac{dV}{dt}$$

$$\therefore \frac{dc_i}{dt} = \omega_i - \frac{c_i}{V}\frac{dV}{dt}$$

Consider eqn. of state: $pV = \left(\sum n_i\right) R_u T$

$$\Rightarrow \frac{1}{V}\frac{dV}{dt} = \frac{1}{\sum n_i}\sum \frac{dn_i}{dt} + \frac{1}{T}\frac{dT}{dt}$$

$$\Rightarrow \frac{dc_i}{dt} = \omega_i - c_i\left[\frac{\sum \omega_i}{\sum c_i} + \frac{1}{T}\frac{dT}{dt}\right] - ②$$

So we get Q dot =to together let us just write Q. over m equals 1 over m σ h.i.v ϖ n i + σ n I capital C_P i dt over dt, so in this we notice that of course the Σ is over I okay I mean I am even dropping that okay but V does not depend on I guess that is common for all these species so I can pull this out of the ∑ similarly dt over dt does not depend on I can pull this out of the ∑ m gets cancelled so considering these I can go with Q dot = to V times Σ H I ϖ i + dt over dt σ n I C_{PI} for the step Q dot / V is =to Σ H I ϖ i + DT over DT σ n I / v C_{PI} what is NI / V number of moles of species I for volume is a concentration okay. The molar concentration so this is Q dot / V equals Σ H i ϖ i + dt over dt Σ CI capital $C_{PI.}$

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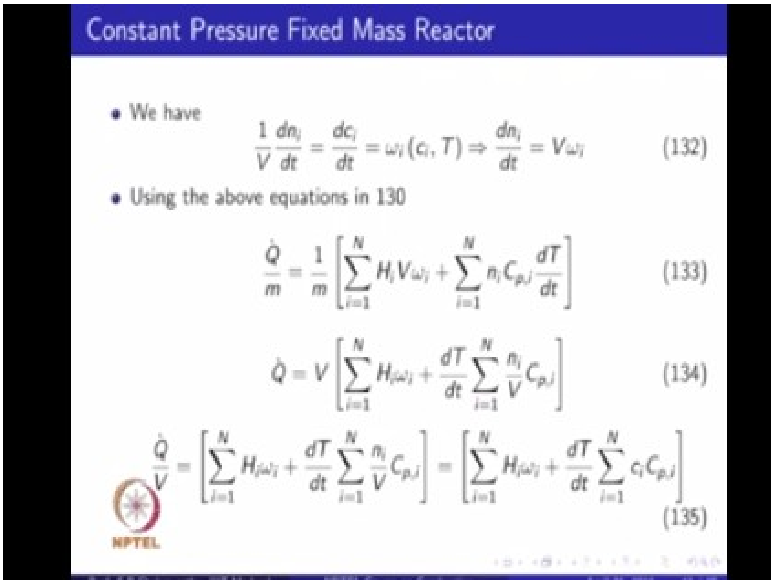

Constant Pressure Fixed Mass Reactor

- We have

$$\frac{1}{V}\frac{dn_i}{dt} = \frac{dc_i}{dt} = \omega_i(c_i, T) \Rightarrow \frac{dn_i}{dt} = V\omega_i \qquad (132)$$

- Using the above equations in 130

$$\frac{\dot{Q}}{m} = \frac{1}{m}\left[\sum_{i=1}^{N} H_i V\omega_i + \sum_{i=1}^{N} n_i C_{p,i}\frac{dT}{dt}\right] \qquad (133)$$

$$\dot{Q} = V\left[\sum_{i=1}^{N} H_i\omega_i + \frac{dT}{dt}\sum_{i=1}^{N}\frac{n_i}{V}C_{p,i}\right] \qquad (134)$$

$$\frac{\dot{Q}}{V} = \left[\sum_{i=1}^{N} H_i\omega_i + \frac{dT}{dt}\sum_{i=1}^{N}\frac{n_i}{V}C_{p,i}\right] = \left[\sum_{i=1}^{N} H_i\omega_i + \frac{dT}{dt}\sum_{i=1}^{N}c_i C_{p,i}\right] \qquad (135)$$

So from here we can get dt over dt equals Q dot / v - σ capital h i ϖ i / Σ CI capital C_{PI} so let us call this equation 1, so what we have achieved here is too right dt over dt in terms of the concentrations and temperature is the temperature showing up here the temperature is showing up okay hi contains the temperature through the sense of length where H i equals Hfi0 + integral 2t capital C_{PI} dt ok and ϖ i = ϖ i of C_I small C_I , T okay that is the same as what we have written there. So we now have a fairly ugly woodye1 or EE for temperature in terms of C_I and key so now you look at how the C_I is going to change right.

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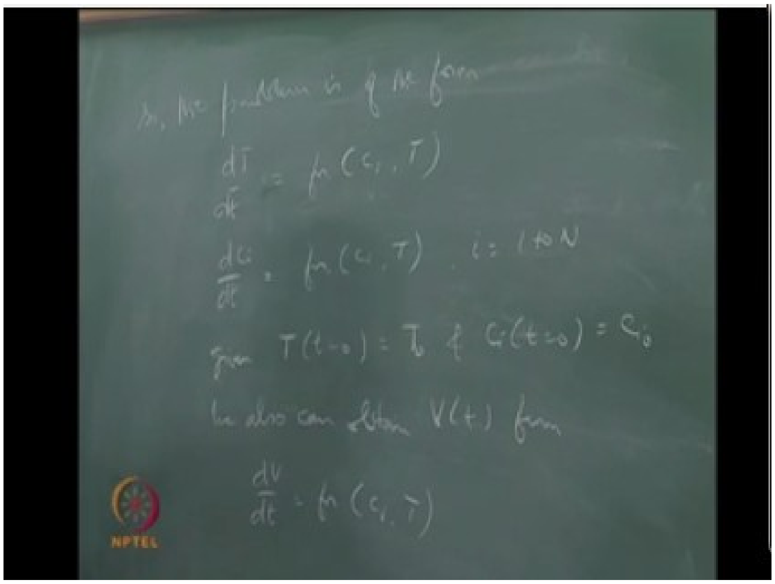

So, the problem is of the form

$$\frac{dT}{dt} = fn(c_i, T)$$

$$\frac{dc_i}{dt} = fn(c_i, T), \quad i = 1 \text{ to } N$$

given $T(t=0) = T_0$ & $c_i(t=0) = c_{i_0}$

We also can obtain $V(t)$ from

$$\frac{dV}{dt} = fn(c_i, T)$$

So you can get your volume so one of the things that is missing here is volume, so we can get the volume V is protein by mass conservation that is there is V equals M / σ c I W_I where W_I is the molecular rate of species I and this is given okay, fix give okay you know you know what is the size of your system from your M from which you can estimate your volume which can be plugged in here I have already told you Q dot is given and so you have an equation there.

See the evolution equations for composition for CI that is obtained by consideration of, what chemical reactions are going on so the C_R is going to change when time so we should be able to get the change in C_I because of chemical reaction what else what else is actually causing a change in C_I? Is molar concentration and molar concentration means number of moles per unit volume okay, so let us suppose that you do not have any chemical reactions but you had a bunch of species inside your piston cylinder arrangement with the concentrations change?

The pressure is fixed with something else the volume changes so if the volume changes will the concentration change, yes as what concentration means okay if everything is concentrated in a small volume then the concentration is high that is what concentration means okay. So many times we just simply forget our English right, so you lose your equations for C_I is obtained by consideration of chemical reactions chemical reaction and change in volume right so dc / dt is ni over V and this is - ni over V^2dv over dt. Now keep in mind we have already noticed that this.

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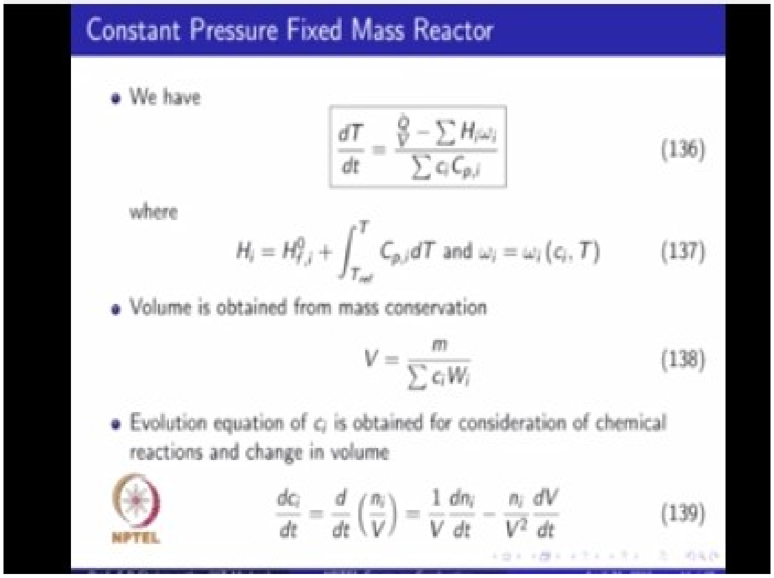

Constant Pressure Fixed Mass Reactor

- We have

$$\boxed{\frac{dT}{dt} = \frac{\frac{\dot{Q}}{V} - \sum H_i\omega_i}{\sum c_i C_{p,i}}} \qquad (136)$$

where

$$H_i = H^0_{f,i} + \int_{T_{ref}}^{T} C_{p,i}dT \text{ and } \omega_i = \omega_i(c_i, T) \qquad (137)$$

- Volume is obtained from mass conservation

$$V = \frac{m}{\sum c_i W_i} \qquad (138)$$

- Evolution equation of c_i is obtained for consideration of chemical reactions and change in volume

$$\frac{dc_i}{dt} = \frac{d}{dt}\left(\frac{n_i}{V}\right) = \frac{1}{V}\frac{dn_i}{dt} - \frac{n_i}{V^2}\frac{dV}{dt} \qquad (139)$$

Is nothing but ωi alright so this is a ω i therefore dc I over dt = to ω i - Ci / v ni over V is C_I so one of the ways gets out there if you know that thinks in terms of Ci, Dv over dt in the next thing we are going to day the constant volume case we can easily see that Dv over dt will be 0 so this does not exist. So you will simply have only this right so I am saying all these things so that I can we can ease the power.

Now this is not easy because we know that ωi is a function of C_I and T alright and then we have to look at what dv over dt is, so consider equation of state Pv =to σ ni times RuT right, so this implies that one over V dv over dt = 1 over Σ n I Σ dni over dt + 1 over T dt over dt right. So if you now substitute here dc_i / dt =to ω I - CI σ ω i / σ c i + 1 over T dt over dt, so this is your second equation.

Now if you are happy with the dt over dt showing up in the expression for dc_i over dt okay because it does not look like a nice set of four test you are free to plug in here plug this in there and make it look a little bit more ugly. So long as you are happy with all the derivatives showing up only on the left-hand side all right it does not make a substitution of this there does not make them dependent on each other they are independent equations they are still independent equations all right so now have two equations and I should not say two equations I take that back this is n equations okay. So this is i = 1 to n is the number of species.

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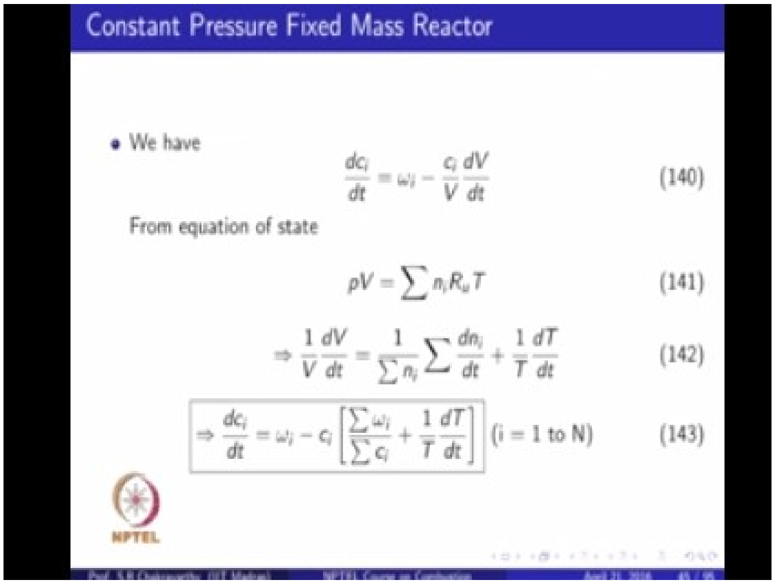

Constant Pressure Fixed Mass Reactor

- We have

$$\frac{dc_i}{dt} = \omega_i - \frac{c_i}{V}\frac{dV}{dt} \qquad (140)$$

From equation of state

$$pV = \sum n_i R_u T \qquad (141)$$

$$\Rightarrow \frac{1}{V}\frac{dV}{dt} = \frac{1}{\sum n_i}\sum \frac{dn_i}{dt} + \frac{1}{T}\frac{dT}{dt} \qquad (142)$$

$$\boxed{\Rightarrow \frac{dc_i}{dt} = \omega_i - c_i\left[\frac{\sum \omega_i}{\sum c_i} + \frac{1}{T}\frac{dT}{dt}\right]} \; (i = 1 \text{ to } N) \qquad (143)$$

So number of species could be quite large for the hydrogen system, hydrogen oxygen system you are looking at maybe thinking about like six to nine species okay including intermediates of course but for something like a carbon hydrocarbon oxidation right, if you are now looking at hydro carbon oxidation by air that means F has nitrogen and then you want to allow for the nitrogen to participate in the reactions by forming oxides of nitrogen okay.

At elevated temperatures you are looking at maybe about 400 reactions and about 100 species okay, so this is this is this is very difficult equations, so you are now looking at about 101 equations to reckon with alright so happy solving yeah but we pose the problem yeah.

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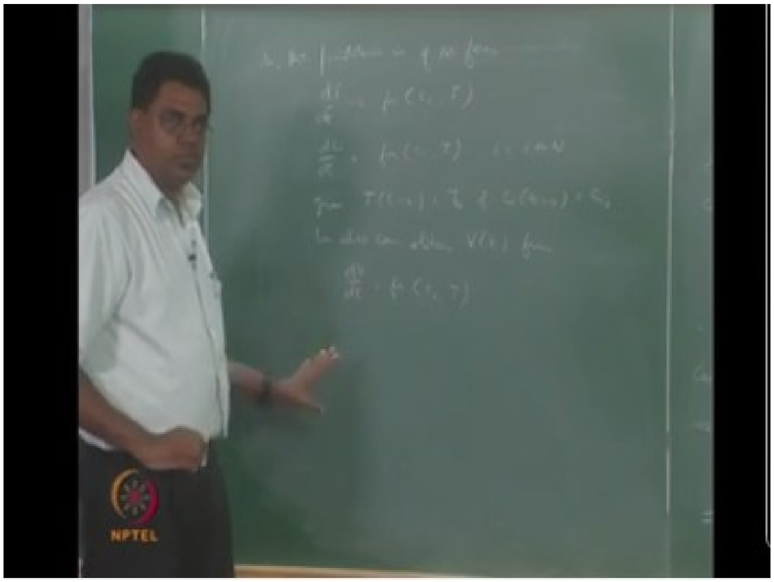

The problem is of the form dt over dt = function of C_I, T dc I over dt is not a function of C_I ,T i = 1 to n given T of T = 0 = T0 and Ci of T = to zero equals C $_I$ not we also can attain V of T from Dv function of CI , T okay once you get your once you solve this you get your CI and t is a function of temper time we can get your volume evolution okay, so this is how we will solve this problem.

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