

**Indian Institute of Technology Madras**

**NPTEL**

**National Programme on Technology Enhanced Learning**

**COMBUSTION**

**Lecture 11**

**Combining Chemical and Thermal Processes 1**

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So we have been looking at a generic skeletal reaction mechanism skeletal because we are only looking at intermediates being present here you are we are oblivious to the presence of the other stable species reactants and products except of course saying that we start with some stable, stable species and you would end with some stable species does thing not be the same as that so this is like a gas phase determination this is a surface termination.

We want to distinguish between these and we want to notice that this is a chain propagation step this is a chain branching step if  $\alpha Z$  is greater than 1 and ultimately we now write a raid, raid equation for the concentration of the intermediate as this where f's actually are essentially factors on the reaction rate constants because these are not this is only skeletal so this is this F F's are the ones that represent the, the rate constants and then the yeah.

And then we apply the steady state approximation and get a expression for the concentration of the radicals intermediates with which we now try to plug in, in the expression or the rate of production of the final product and we get this expression right so what we mean by a chemical explosion is when your  $DCP / DT$  goes to infinity and that happens when the denominator goes to 0.

And the denominator can go to 0 only when  $\alpha$  is greater than one and as far as great as for greater than 1 indicates a chain branching situation that means you now have a, a creation of radicals more, more, more radicals in the second step right so this is what we have seen so far the

additional thing that we have also began to notice so far is question is what happens as you now change the pressure right so as you change the pressure we expect that the surface termination should actually try to come down because the molecules are busy colliding among themselves rather than colliding on a surface okay.

The surface location is fixed its surface area is fixed whereas the molecules are actually trying to collide with each other as you increase the pressure more than they actually collide with the surface the same not same molecules the probability of collision among themselves is more when compared to collision with a with a surface therefore the surface termination is actually going to decline as you, as you, as you increase in pressure.

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So if you were to now try to plot how this, this is going to happen so that is suppose that you plot your various  $f$ 's that are participating in this equation with pressure so let us now say we have a pressure showing up we expect that  $F_S$  should decline like this and on the other hand for a similar reason if  $G$  should actually start increasing as you increase in pressure because you now have to have more and more gas phase determination happen as increase as the pressure increases relatively speaking.

Therefore you are now going to have a curve for FG that goes like this now put these two I am sorry should have looked at so you need to have the gas phase go up like this in fact there is no reason to believe it would actually ever flatten out the way because as you keep on increasing the pressure the FG should keep on increasing pretty much nonlinearly and therefore we now expect a FG to go like this and then we are now looking at  $f + FS$  and FG together you see because they are termination reactions.

Therefore your  $FS+FG$  is now going to go like that so as you increase in pressure initially FS comes down and therefore  $f + FG$  comes down but as you as you as you increase in pressure further FG grows up even though FS comes down and that makes up for it and therefore the  $FS$  plus  $f$  keeps increasing further now this together is now balanced by the  $FB \alpha^{-1}$  right so the question is how does that go and we expect that you now have to have a production of intermediates because of chain branching and that mean, and that mean not necessarily grow with pressure forever right.

So that means we expect that this should actually go more like that right so this is now  $FB \alpha^{-1}$  that means as you keep on increasing the pressure the chain branching need not happen forever so it begins to level off after a point but the interesting thing here is the question is where as this matching this right and graphically we can now see that  $FS+ FG$  now is having, having the same value as  $FB$  times  $\alpha^{-1}$  here and here.

So there are two pressures at which you now have this match happening that corresponds the denominator going to 0 which corresponds to the rate of production of products just exploding right so if you were to now look at how the, the  $DCP$  over  $DT$  is going to fare with pressure right we now try to say let us just bring this downright strictly speaking I need only one half of the positive domain so good a good draw ay, ay axis somewhere up there allowing for some space at the bottom as well.

Because we are looking at net production of products which could go negative so what does what this means is we are now looking for some production of products that stops from somewhere we

do not exactly where to start let us say some pressure lulu pressure and then it goes up to infinity right and in between hear you now start with a negative infinity because the denominator is now beginning to flip sign okay.

So you now having if you now go here you now have  $FB$  times  $\alpha^{-1}$  greater than  $f_{s+}$   $f_t$  so you just had a flipping of science so it starts from negative infinity goes all the way up and then comes back to negative infinity again and you now have a flip flipping of signs again right so what is going on we are now saying that at low pressures you have a significant, significant surface termination and, and then there is some point as you now keep on increasing pressure that the intermediates are beginning to actually get produced by chain branching much more than the rate of termination okay.

Because the determination is actually coming down as you increase in pressure so you are producing more and more intermediates and creating an explosion and the other time so and then you now get into a explosive regime and you, you know the other time you are not going to have an explosion is when the reverse happens that means you now have lot more gas phase termination right.

And so the gas phase termination keeps increasing but the production is not increasing that much okay so, so this is this is now tapering off and then you now have a reversal again of  $f_{s+}$   $f_t$  exceeding  $FB$  times  $\alpha^{-1}$  so these two pressures now are they looking at pressures essentially right that means we have not really bothered about what, what we are doing with temperatures so the reason why we are doing that is because with pressures.

We can think about collisions increasing or decreasing or surface curves determination declining in importance relative to gas face termination and soon all these things are pressure related we have not thought about temperature so it is as if like we have kind of fixed a temper so the corresponding picture if you were to now bring in temperature here and pressure were to be plotted over there would be to now look for a curve that would go like an inverse S where you were to fix your temperature at some point at any point okay.

And then you will find that this is your let us suppose that this is your P1 and this would be a p1 okay and then you have a P2 here then this is your P2 that means for a given T this mechanism is able to does this mechanism is able to show that there would be what is called as to explosion limits so you have a explosion regime here and no explosion on this side or in other words in the PT plane in the PT plane this line marks a boundary which corresponds to crossing over to explosion all right that is to say if I were to fix my temperature and keep going up in pressure that is like saying go horizontally in this direction.

I now cross an explosion point and get into an explosive region until I get to P2 when the gas phase termination begins to predominate over the chain branching and therefore I cross into the no explosion limit all right and this of you obviously can actually move back and forth as you change the temperature yes please to infinity nothing yeah I am sorry thank you was there a cause of confusion for about 20 minutes we should have remedied it long ago right so okay so we now can explain this right so this is this is the famous s-curve all those alerts and inverted S but it is okay.

We will just call it as we always name things based on what we what we familiar with so then the question arises hey the s-curve also has another point P3 that is not explained by this one here okay so how did he give the S-curve this is an experimental observation that means you now take what is this P & T that we are looking at those are the initial pressure and temperature so you now take a reactant mixture at a particular pressure and temperature okay.

If it were to be located somewhere here that means it is not got an explode chemically explode but if you were to take a chemical mixture and get it up to a certain pressure and temperature that would locate itself somewhere here that means it is going to go through a chemical explosion alright that is what it really means or you could take a chemical mixture and then keep it over here your  $DCP /DT$  is not going to be infinity and then keep on increasing your pressure and then you are going to go through an explosion.

As you now cross that curve that limit and if you now keep doing this experiment you will find that this you, you get this curve for different temperatures you do this and you get you get this

curve and the curve is actually an inverse S shape whereas what we have done so far can explain only about two pressures to two limits okay it does not explain the third limit that is also observed okay.

So how are we explain the two limits it is essentially looking at chain branching versus a surface termination or chain branching where is it say gaps face termination okay make sure is that the, the light at then as the inverted S-curve what will happen then you have to look at you then, then you go a little bit further you have to look at stability so what we have done is only to look at the equilibrium okay.

So you have to put up and then you will find that if you if you feel if you here then I did I do not want to get into this so strictly speaking if you are like in this stability you will draw like adopted line for this and a solid line for this and so on so the solid line indicating that it is stable at the point where as the dotted line indicates it is unstable okay so unstable or stable really means that depending upon which way you put it okay you put out into the no explosion side it will not explode but if you put up in the explosion site it will continue it explode and so and so on that is that is if it in stable and, and, and so on.

So let us not let us not get into that, that is getting it getting further out okay so fine we will just keep it that way the question then is what about the third limit right there are there are a quite a few explanations for this one of the explanations that I would like to in fact this, this is, this is observed for let  $\text{H}_2\text{O}_2$  system right observed, observed for okay.

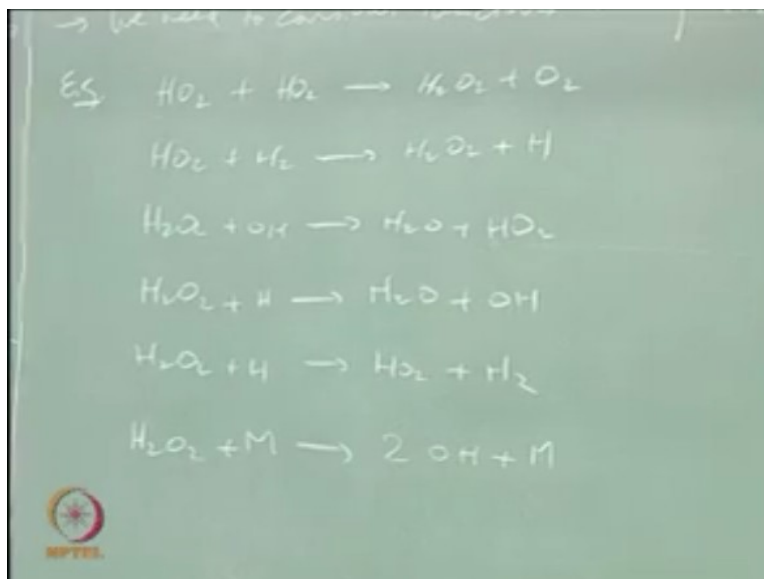
So S-curve as observed for the  $\text{H}_2\text{O}_2$  system so that the question is about the third limit there are a couple of two or three theories about this all of this act actually acting with each other one of the things that we have been talking about when we are talking about changing pressure is the competition between uni-molecular to by molecular reactions or by molecular tutor molecular reactions.

So when you are now looking at very high pressures then the molecular reactions become very important so the question then is you now look at this scheme that we already had depicted

earlier for  $\text{H}_2\text{O}_2$  system a basic 9 step reaction scheme okay where you now have a alter molecular reaction step so this is now going to give rise to a, a new intermediate as opposed to OH and OH alone you now have a  $\text{H}_2\text{O}_2$  that also has a surface termination and a gas phase termination you see so the, the molecular reaction giving rise to a new intermediate is it is, is one of the mechanisms.

That explains a very high pressure limit this is this is 1 1 idea the second idea is you now also get into a  $\text{H}_2\text{O}_2$  cycle that means this at this time we are not really bothered about the formation of hydrogen peroxide right so the there is a we find a we find a third limit in the experiments right so this is some due to importance of thermal ocular reactions at very high pressures so the production of HO to H to do is say is a hydro peroxide a chill so at very high pressures you now have the importance of production of hydro peroxide radical and the second idea here is we need to consider reactions involving, involving  $\text{H}_2\text{O}_2$  as well.

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So example I am saying example because this is not exhaustive okay as a matter of fact we have about nine reactions herein reality you might have to consider something like 40 reactions and maybe nine species okay so the nine species here would be like  $\text{H}_2\text{O}_2$  HO OH there is a  $\text{h}_2\text{o}$   $2\text{h}$

$\text{H}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{H}_2\text{O}_2$ ,  $\text{H}$ ,  $\text{O}_2$ ,  $\text{O}_3$  okay so we may have to consider as many as nine species and about 40 reactions but the idea basically is what is the least number of reactions and species that we need to consider to explain a certain phenomenon that is the way we would approach chemical kinetics all the time alright.

So that is a reduced mechanism that we need to adopt so here for consideration of  $\text{H}_2\text{O}_2$  we may have to say let us say we now have  $\text{HO}_2 + \text{HO}_2$  gives you  $\text{H}_2\text{O}_2 + \text{O}_2$   $\text{HO}_2 + \text{H}_2$   $\text{H}_2\text{O}_2 + \text{H}$   $\text{H}_2\text{O}_2 + \text{OH}$  gives  $\text{H}_2\text{O} + \text{HO}_2$   $\text{H}_2\text{O}_2 + \text{H}$  gives  $\text{H}_2\text{O} + \text{OH}$   $\text{H}_2\text{O}_2 + \text{H}$  gives  $\text{HO}_2 + \text{H}_2$  and the  $\text{H}_2\text{O}_2 + \text{M}$  that is a gas face termination gives  $2\text{OH} + \text{M}$  you see there are a couple of things that I would like to point out with but a new intermediate that could be formed first of all if you want to look at what happened to the  $\text{HO}_2$  in this reaction step.

We now said  $\text{HO}_2$  is some getting produced by the stirrer molecular reaction that would be pretty important at high pressures number one second thing how does it get absorbed it has a surface termination and it has a gas phase termination the gas phase termination is  $\text{H}_2\text{O}_2 + \text{H}_2$  which is the stable reactant produces a stable product water plus  $\text{OH}$  but there is an alternative path right.

So you could now say  $\text{H}_2\text{O}_2 + \text{H}_2$  produces  $\text{H}_2\text{O}_2 + \text{H}$  all right now this is another chain branching right and it now produces a new intermediate  $\text{H}_2\text{O}_2$  which could now get consumed in a succession of steps and notice that this for example is a reverse of that okay so has  $\text{H}_2\text{O}_2$  is being produced it could equilibrium with its, its consumption in a reverse reaction right so you could have a second set of intermediate production that is possible here as a, as a secondary route to a termination of a particular intermediate at a high pressures.

And of course the last possibility that sets term, term is a thermal that is it is not really a chemical explosion so not necessarily just a chemical explosion the third, third thing is the third limit could be thermal in nature that is to say reaction rates are shoot up so high so high and these reactions are the exothermic keep in mind so when you now have exothermic reactions that are happening very fast right then you have a huge rate of generation of heat right that could actually increase the temperature.



And as the temperature increases the reaction rates increased further right and as the reaction rates increase further the, the heat release rate increases further as well and, and so on right so that is that is what is called as a thermal runaway and so under these conditions under these conditions or the steady-state approximation is not valid in other words you could not hope to explain the third limit particularly within the within the framework of a steady-state approximation okay.

So you have to account for the thermal runaway in explaining the third limit so effectively we are saying essentially that a mechanism like this is essentially taking care of like one kind of intermediate if you now have multiple intermediates you might have other limits as seen in, in H<sub>2</sub>O to scale into the mechanism plus a additional possibility of H<sub>2</sub>O<sub>2</sub> formation keep in mind.

Another aspect is the term molecular vs. by molecular which becomes important at high pressures so these are the things that actually constitute the third limit is what we can say from here the next thing that we want to now say when we are now beginning to talk about thermal is where do we go from here.

So let us now look at the possibility of combining chemical and thermal processes right in the very first class we talked about combustion is having convection and diffusion and chemical reaction okay convection is about the flow diffusion is about mixing of species and then you have the chemical reactions anyway and of course we said that we are essentially looking at typically fast chemical reactions right.

When we set fast we are essentially looking at the chemical kinetics so this is something that we did after we did the chemical equilibrium that would give you the adiabatic flame temperature so we done chemical equilibrium all right and then we have done chemical kinetics the chemical equilibrium gives you what the adiabatic flame temperature should be before the final products assuming that they exist in equilibrium chemical kinetics.

Basically tells you what happens to the rates of reactions when they now depart from equilibrium n states that means you start from reactants and then now you want to proceed towards products

what's the rate at which you are now going to go from here to there right as you now depart from an equilibrium initial state and, and proceed towards a equilibrium final state you are now departing from this equilibrium and going towards another equilibrium right all along when we are doing chemical kinetics.

We are not really worried about changing temperatures you are saying that a reaction rate is equal to a rate constant times concentrations raised to their stoichiometric proportions the concentrations will depend on pressure but the rate constant is the one that will depend on temperature in an exponential fashion right so if I were to now look at a system of reactions where multiple species are involved and I want to actually keep track of rate of production of a particular species in all the reactions put together it could be getting produced in one reaction getting consumed another reaction.

I now have to sum over all the rates of production of that particular species in each of the reactions across all the reactions and then I have to keep and keep track of what is the rate constant for each of those reactions times the products of the concentration in those reactions raised to their respective stoichiometric coefficients and so on and in all these things I now get a system of  $E$ 's right which, which are for each of those concentrations the rate of rate of production of those species concentrations right  $dC_i/dt$  over  $DT$ .

And then what we did was well we say are very, very nonlinear do you have an initial value problem all right but you have to now solve these things simultaneously these are stiff equations because you now have very small chemical times that you have to take care of and so on therefore we said if you are if you feel if you are applying state approximation you can now set a bunch of  $dC_i/dt$  is equal to 0 because all of them are intermediates and keep track of only the stable species reaction rates or production rates.

Another way was a partial equilibrium approach where we said that those reactions that are involving intermediates could be assumed to exist in equilibrium with each other because they are happening very fast when compared to the final step right he thereby we now say we can replace the  $dC_i/dt$  for those species by algebraic equations through their equilibrium constants

so these are things that we would try to play with under different conditions to, to, to simplify our equation set all along not bothering about what happens to the temperature.

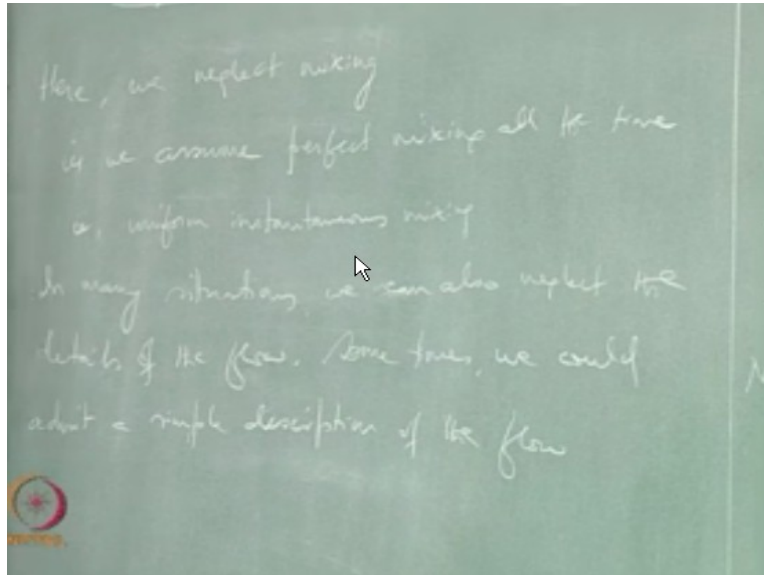
In other words if you now have a set of reactions that are happening they would give out heat and take out Heat okay whenever really bothered about it and we did not worry about what is the net heat that is produced in this set of reactions and while you are doing combustion we are expecting heat out as a net thing there are some reactions that are going to take away heat because the day they are endothermic but largely we are expecting that many of you many reactions are going to put out heat right so when you in high school right these simple reactions and then you put a  $\Delta h$  at the end okay.

We never did that when we did chemical kinetics we did that when we were doing thermodynamics then we drop that habit because we are now looking at how fast we want to go we did not worry about what is, what is the heat? That is going to come right now what is the problem why should we have worried about it we cannot be just worried about the read rates alone should not we should we worry about the heats along let that come along the answer is when the heat is going to come along.

It is going to heat up the place and when he when it heats up the place the temperature is going to change the temperature changes the reaction rates are going to change right and the reaction rates are going to change the heat release is going to change and the temperature is going to change and so on so the real problem is in taking into account not only the chemical kinetics but also the changes in temperature because of the heat release that happens in these chemical reactions right.

This is still not bothering about the flow and mixing we are still not really looking at a full-blown combustion problem but we go take baby steps we do equilibrium we do depart from equilibrium and look at how fast then we start worrying about what is happening to the heat that comes along and the changes in temperature that that will that will influence the how fast thing again right so that is the next step that we want to do so here we neglect mixing right whenever you neglect something it does not mean that it does not exist okay.

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You are you are taking it for granted right so that is what you do with your parents and teachers are you neglect them not because they do not exist right you just take that for granted so here again what you what you are doing here is we are saying that it's all perfect everything is fine no problem my parents always allow me so what is the problem so, so it is like that is we assume we assume perfect mixing all the time that is again to, to, to, to further elaborate we say uniform instantaneous mixing right uniform to cover space and instantaneous took over time the means at all times in all places you expect mixing to happen uniformly therefore any species that is there is there everywhere instantaneously okay.

So if you now have a mixture of species reactants products intermediates all of them get mixed instantaneously everywhere in the region that we are interested in this is what we are basically assuming right the means you do not worry about spatial concentration gradients and this is going to become very important when we start thinking about mixing in greater detail okay spatial gradients in concentration or the ones that are going to drive mixing.

We now suppose that you have a spatial uniformity all the time that means if you now have a change in the concentration that that, that leads to a instantaneous mixing so that the

concentration is you firmly spread in space so that you do not have any special concentration gradients that will drive the mixing okay is it okay is it okay to do this but there are conditions under which this will be very useful for us to think about okay so for example what, what you are basically saying is the mixing has to be so fast right now typically mixing is not really as fast as chemical reactions.

When you are now looking at combustion kind of chemical reactions right so how does it make sense well why so not I take my hand and put in there and then stop mixing as vigorously as I can yeah sure yes of course you do, do not do this because you are going to get, get your hands burnt you can put a spoon and start stirring right so this, this is very typical I mean what you are talking about now is to promote mixing through things like turbulence okay.

So if you now have like a highly turbulent situation okay where the turbulent mixing is going to promote a homogenization of this of this mixture okay instantaneously then we take advantage of that and we think the turbulent combustion is very complicated but there are regimes of turbulent combustion which could which we could take advantage of there is like so much turbulence in there that it just smears out everything and then the mixing is complete.

We do not have to worry about it right so that is a kind of approximation that we could do that we could apply to many practical systems as we will see right so we can also in many are in many situations in many situations we can also neglect the details of the flow videos of the flow that means you either do not have a significant flow at all through to talk about okay in relation to what is what we are thinking about that is chemistry and, and temperature, temperature gradients.

And so on or the flow is so complicated that we do not want to worry about the details case it is always like I come either like you do not have when you say you neglect mixing that could have been fine when you did not have any mixing to worry about but what we are basically saying is there is a lot of mixing that is going on that we do not have to worry about it okay similarly when we say we can neglect details of the flow then the means either you do not have too much flow okay.

That is good or you have so much flow that that's going around it is very difficult for you or would you make so much flow turbulent flow right so when you now say turbulent mixing it is basically caused by a flow turbulence is essentially a, a fluid dynamic situation the mixing that comes with it is accompanying the turbulence right so in a sense when you're now trying to put these two together they go together the assumptions basically kind of go together if you are thinking about a intense turbulent combustion situation.

Then the flow field is so complicated that we do not want to worry about it neglect its details and it also facilitates a more instantaneous mixing hat we do not have to worry about it okay so many sometimes, sometimes we could admit a simple description of the flow in a way that does not really affect our focus on looking at the coupling between chemical and thermal reactions thermal processes right chemical, chemical reactions in the heat.

So essentially we are looking at where we are now taking a magnifying glass and looking at only a coupling between two things the chemical reactions and the thermal feel that it creates okay anything else that comes around it is something that we want to neglect and look for situations when we can neglect it right so if you can allow for a simple description of a flow in some condition some situations right that does not really come in the way four looking at this combination then we could admit it right.

So let us just look at when are those conditions that are possible right so the balance here so the balance to be considered here is between, between production or consumption of, of, of species in chemical reactions and the thermal energy associated with it right obviously we want to do this in a region that is that is meaningful when you now say you cannot you want to have instantaneous mixing it is possible only in a small region right.

So we would now want to confine our attention to in a region okay in the region such as a, a reactor so typically a reactor is a terminology that is used by chemical engineering people the aerospace people call it a combustor okay but essentially the chemical engineering people are looking at like a broader set of chemical reactions that are possible than just combustion kind of reactions.

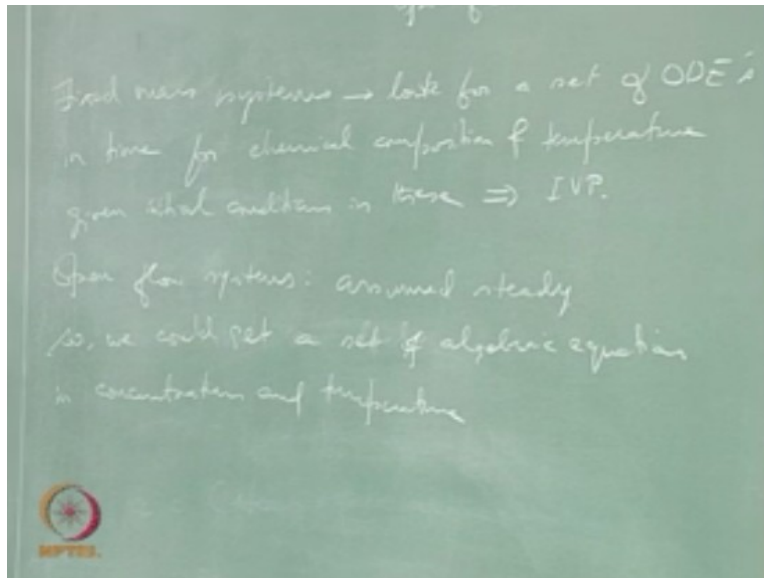
So they would call it call a region where they want to have chemical reactions happen as a reactor okay and then we are looking at a intense mixing happening in a region that we want to call a reactor okay so what are the typical kinds of reactors that we want to look at that will facilitate handling this restricted set of conditions is a question.

Broadly we could say brought me we can say reactors are like fixed mass reactors or open flow all right that means you are now taking a certain mass of reactants allowing for the reaction that happen and the reactants now become products but the mass does not change right mass is conserved in a chemical reaction anyway therefore the mass of the product should be the same as the mass of the reactants or the mass of the system that we are talking about should remain the same through the reaction right.

So this is now looking at a fixed mass system on the other hand you could have open reactors that means you now have a inlet and an outlet yeah so you now have reactants come in this way go through some reactions and get out as products so it is sort of like a open system right and it is a open flow system right so you cannot really talk about a fixed mass you might be able to talk about a fixed mass flux or a mass flow rate right.

When you now talk about I fixed mass flow rate that means implicitly you are think in like a steady state so on a steady state basis if I now keep in a flux of reactants coming this way a flux of products go out that way and there is like a intermediates that are formed and, and get quenched by the time you have the products that go out right all of this is happening all the time so that is like a steady state situation as opposed to that a fixed mass reactor is like a batch process where you now take a certain mass of reactants.

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And you have to allow for things to change in time from a set of reactants to set of products right obviously that is not steady state things change in time okay so we are essentially looking at fixed mass systems right we look for a set right in time in time for a chemical composition and temperature and temperature okay previously when we were worried only about chemical kinetics as if the temperature was fixed artificially by us externally there is possible you could actually have a chemical, chemical reactions happening in a bath that is maintained externally by a constant temperature right that is what we were thinking earlier on for a physical system okay but here in addition to the chemical composition.

So when you say composition we are now talking about let us say let us let us fix it we are now talking about molar concentration see  $I$  for the is species  $I$  going from 1 to  $n$  for  $n$  species right so in addition to the concentrations molar concentrations of chemical species that will give the chemical composition as a function of time we also have to track the temperature as a function of time that means you need to have a ordinary differential equation in time for temperature as well that is like  $D \text{ capital } T$  over these small  $T$  okay.

There must be a rate equation of sought for, for the temperature change in time okay given initial conditions in these right so this would actually be a initial value problem what you will find is the rate of the rate of reproduction net, net rate of production of each of the species whose



composition whose concentrations that we are interested in will depend on the concentrations of lots of other species and temperature.

And similarly the rate of change of temperature the equation that we write for the rate of change of temperature with time will involve the rate of production of other species which in turn means that it will involve the concentrations of other species so you are now looking at a couple set of okay that is each equation in the set has variables that are present in most of the equations the means you have to solve all the equations simultaneously okay.

So that is a that is one initial value problem for the entire simultaneous set of equations on the other hand if you now look at open, open flow systems we assume them to be steady, steady that means we just said let us not worry about unsteadiness that means we do not worry about evolution of the concentrations from reactants to products in time and, and correspondingly the temperature that is also associated with it okay.

That means we do not have to have would EES we could simply look for algebraic set of equations you are in a crude sense we will look at the details lot more carefully as we go along but in a crude sense it is a is essentially saying let us now throw weight terms that involve  $d/dt$  okay any change in anything with respect to temperature time we let us get rid of it you now set it equal to zero at steady state then  $a_0$   $de$  with the first derivative a first order  $o$   $de$  with the first derivative thrown in you do not have any differential equation anymore right.

So effectively you will you, you could reduce your system of equations to a simultaneous algebraic set of equations right so we could so we could get a, a algebraic set of equations should say set of algebraic equations, equations are in concentrations and temperature right okay why am I saying we could is if you do not consider any spatial variation okay now what we looked for avoiding earlier is a spatial variation in spatial gradients in concentration if you assume that spatial gradients and concentration do not exist.

But let us suppose that you now have a, a duct that could be a convergent divergent nozzle where reactions are happening like for example at the towards the exhaust of rockets okay so

when you now have chemical reactions that are happening in a combustion chamber and pushing into a convergent divergent duct you have a flow so if it is possible for you to have a simple description of the flow and the flow changes as we go along because of the convergent convergence and divergence and so on.

That is going to distribute your temperature and, and species in a convective manner not on a diffusive manner okay diffusive is what we are trying to avoid in our inner formulation but you could look at a variation in space purely because of convection by admitting a simple description of the flow so or we could we could get Oh des again but this is not Oh des in time but Woody is in space okay so des in space in 1d space that the reason why it is 0 de s space for concentration and temperature concentrations and temperature, temperature by admitting a simple.

Let us say quasi 1d flow description alright so it is possible for us to actually try to do a few different things within this framework effectively okay and we will now for different many of these different conditions we will now be able to get and time worries in space or algebraic equations which are simply taking into account only the chemical reactions.

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## Combining Chemical and Thermal Processes

- Assumption - neglect mixing ( or mixing is extremely good and instantaneous due to turbulence etc.)
- Assumption - neglect the details of the flow.
- Fixed Mass Reactor - Set of ODEs in time for chemical composition and temperature given their initial conditions (IVP).
- Open Flow Systems - Assumed Steady, algebraic equations for concentrations and temperature or ODEs in 1D space for concentrations and temperature by admitting a simple quasi 1D flow description.



The mass production of species or mass depletion of species and the heat release that there is associated with them doing an energy balance of that okay we will continue from here on Monday.

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