Fundamentals of Combustion (Part 2)
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Lecture – 64
Mechanism of Soot Formation and Introduction to Liquid Fuel Combustion

Let us start this lecture thought process. If you aspire for better tomorrow start working on it now using all the resources at your disposal. So, if you look at in the last lecture we basically initiated discussion on the Soot formation mechanism; how the soot being formed. And today we will be looking at little more details and keep in mind that whatever the mechanism I am trying to discuss with you is not ultimate one.

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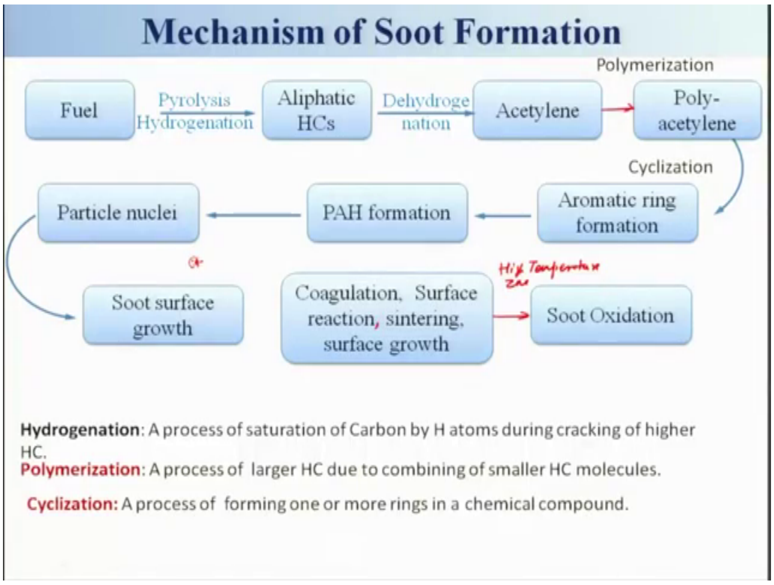

Hydrogenation: A process of saturation of Carbon by H atoms during cracking of higher HC.

Polymerization: A process of larger HC due to combining of smaller HC molecules.

Cyclization: A process of forming one or more rings in a chemical compound.

This is just a one way of looking at thing that I must tell you right because, this is very very complicated in nature and people have not understood the actual mechanism, it will take more time. But however, I will be talking about is basically some kind of general mechanism. If you look at the fuel, fuel will be subjected to pyrolysis.

Pyrolysis means that means, it will be you can say thermal heating kind of thing process. In which the higher hydro carbon will be converted into lower hydrocarbons right. And generally in the absence of oxidizer that is the pyrolysis, but however, there might be some kind of a oxidizer which will be leaking into it. But in case of diffusion flame, generally leakage will be nearby the flame surface not far away from the flame surface.

So, there will be also some hydrogenation. So, hydrogenation is basically a process of saturating the carbon right by the hydrogen atom during cracking of higher hydrocarbons right because, some hydrogen will be coming and attaching.

And then you know so, that the carbon will be saturated kind of thing, that both will be going on parallely. And then you may get in something aliphatic hydrocarbons right, you may get or may not get the kind of things. So, therefore, there will be hydrogenation will be also taking place. I have given in a very linear way this process what I am describe, but that do not that way; dehydrogenation means basically it will be removing the hydrogen atom from this aliphatic compounds and making the way for the going for the double bond or the acetylene kind of structures right. And, acetylene generally people consider is to be the main things for the initiation of the soot formation and acetylene will be basically also polymerize.

Polymerization is the basically the process of forming the larger hydrocarbon due to combining the smaller head molecules right, that is the basically polymerization. And due to this polymerization you may get some polyacetylene kind of features, the process you can say this way right. And, then it will be also when you are doing this poly acetylene and some other things will be then it may cyclization and it will be basically cyclization the process of forming one more or more rings in a chemical component. Because, the ring structure is very important like your benzene you know there is a ring structure right. And, that gives to the aromatic ring formations right because, of the cyclization and then you will get the patch formations right and patch is a very important precursor for that and this patch is basically what poly aromatic hydrocarbons right.

And this patch will be and now converted into the particle nuclei and this is the initiation of the soot particle. If you look at all our gaseous phase is taking place and then from that you are getting a solid that is the soot nuclei of the particle nuclei means initiation. And, then if this nuclei the soot there will be some growth of the this soot particle which will be taking place. If there is a soot here right, let us say there is a soot here then the some vapour will be coming and then coming over here getting cooled right. And, then the surface will be growth, there will be surface growth right will be there. And, then beside this when this soot are born there they can come in contact coagulate right, join each other. There might be making formation because of high temperature right, they join together there might be sintering also right.

There are several things which will be taking place, all are there will be surface reaction which will be taking place and beside this there will be some also surface growth all are taking place parallely right. And then when this is taking place there can be various processes which are taking place and different sizes will be there and this soot will be passing through some very high temperature zone. And then it will be get oxidized; that means, you know the size will be reduced again right and it will be passing through that.

So, this is the whole process one can say, as I told earlier that this process is basically I have shown in a very linear fashion, but it is not the case. Why? The nature is not linear, it is all non-linear in nature. So, what it will be trying to do how the particles are formed other things is a matter of research and debate, discussion. So, it is just the model, but I will be showing you little more specifically.

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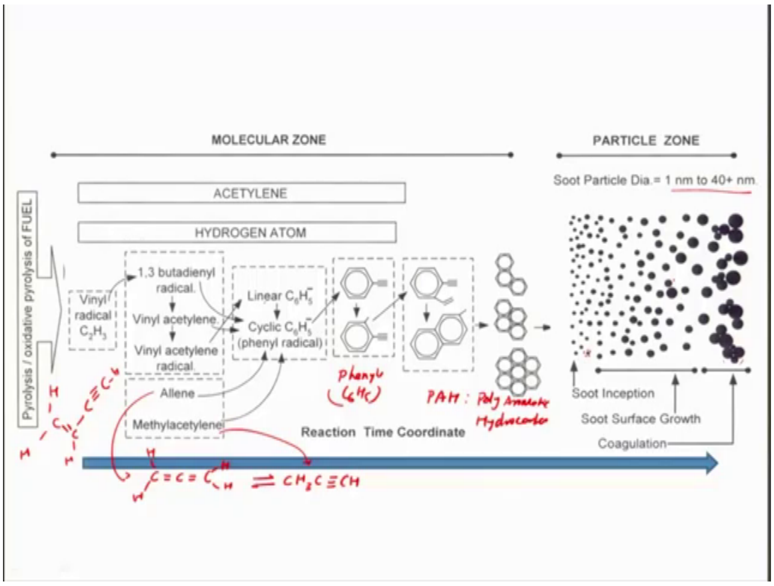

And let me tell you that how it can be this is again another model. If you look at this is the as I told this is a pyrolysis or you can say oxidative pyrolysis of fuel right and basically oxidative means there might be some kind of oxygen which will might be there. And then there will be vinyl you know radicals which is will be there it will be in a same it can be converted into 1 3 butadienyl radicals right. And then it can be vinyl acetylene kind of structures right if you look at these vinyl acetylene structure it will be looking like that.

So, this kind of thing vinyl acetylene radicals will be looking like that and then there will be also allene being formed. Allene structure will be looking like that. Let me show you that this is basically C C double bond and then C this H and H and this will be and this is can be converted into basically methylacetylene right, it can be converted into that this can be converted into methyl acetylene which is basically CH 3 C triple bond kind of things right.

And these are you getting then it will be cyclize after this you know once it is formed to this form this is basically methyl acetylene then it will be linear it will be 6 5 kind of thing H 6 it will be this thing. And, after that this will be ac once this is this can get into this vinyl acetylene C 6 H 5 or it can go to cyclic C 6 H 5 kind of phenyl group it can come into and allene can get into this here or methylacetylene can also convert into C 6 as any other root it can take.

And then once it is come then it will be basically phenyl things which will be formed here right C6H5 phenyl group and then that will be again joined together polymerization will be taking place. And this is basically patch this is patch is being formed. The patch is being joined together you know this is a well phenyl group they will be joining together and putting this patch.

Patch is basically poly aromatic hydrocarbons. And once it is formed then what is all you will get the soot particles right and soot particle that is the inception of soot particles right. And, till now whatever is happening is in the molecular level right this is known as molecular zone right, you can say there will be some zone where it will be taking place. And then after that this is you can say the particle once it is being formed there will be also surface growth. If you look at this particle as it is moving there is a surface growth and it is increasing and then it may come in contact you know like a surface growth will be continuing and then they may come in contact they may be sintered, then there might be surface board. It may increase its size right coagulation will be taking place and all those things you will get you know particle size Soot will be 1 nanometer to 40 plus nanometer order you will be getting right.

And these particles sometimes the smaller particles is basically known as the incipient soot and some clean Soot. That will not be radiating much, but whereas, this larger one it will be radiating because it is a black in color. And then it will be radiating the more amount of it keep in mind that the larger particles will be of course, we can see. But the smaller particles is a very very dangerous than the larger particles particularly in the CNG and other things you know the particle size will be very very small and that will be more reactive than the larger particles right.

So, therefore, we are getting the asthma and other problems is being enhanced more because of use of CNG gas you know we are saying we have overcome the problem of the diesel soot. But however, we have now put some soot which you cannot really detect it. So, this is a more dangerous than the this thing that you should keep in mind. Let us now get back to the jet diffusion flame.

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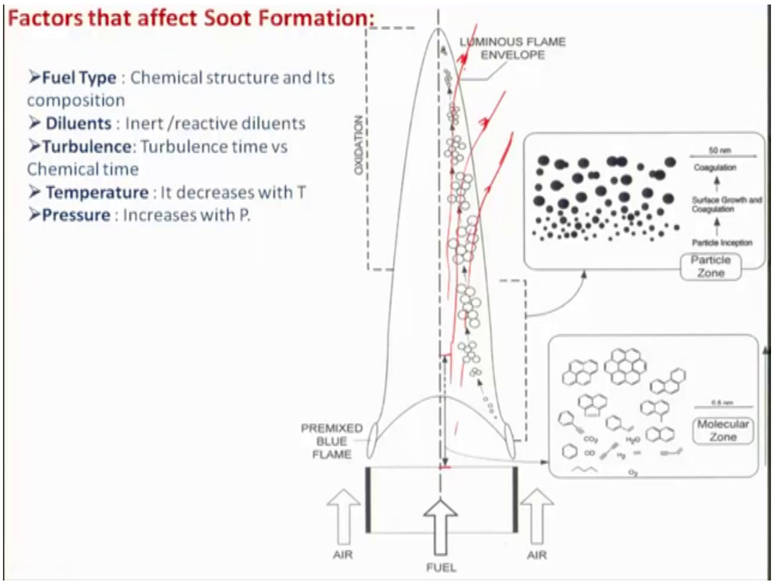

Factors that affect Soot Formation:

- **Fuel Type** : Chemical structure and Its composition
- **Diluents** : Inert /reactive diluents
- **Turbulence**: Turbulence time vs Chemical time
- **Temperature** : It decreases with T
- **Pressure** : Increases with P.

What is really happening? If you look at this is zone is basically the molecular zone right. Where all these things will be taking place polymerization and then you know all the processes I have already discussed like hydrogenation, cyclization, polymerization all those things are taking place and the patch is being formed right. And these are the inception point this is the premix flame, if you look at there is nothing will be happening here.

But here it will be taking place and then the particles generally the this region is basically the molecular zone right. But however, as it goes on this will be particle size will be increasing and these are the particles zones and of course, in this temperature because it is not that way I have shown it can be depending on the stream line. Like if I say this is the stream line is going like this way the particle will be moving in this you know it will be passing through the flame. And some stream line will be moving this way right.

So, therefore, that will be taking away the particle through the flame and then it will get (Refer Time: 12:40) some can go straight right some can go stream line can go straight also right. So, that is this is basically high temperature zone. So, this is known an oxidation if you look at particle size again decreases because of oxidation right. So, more it will remain is the go through the flame and then temperature higher zone.

So, then particle size you can reduce right. So, this particle size if you look at we will have to see that. What are the parameters that govern the particle size and its distribution? And I will just discuss some of them already we have discussed that is the type of fuel right, we have seen that aliphatic is having the more prone to the alkanes kind of things. And, higher hydrocarbons are more prone to the soot than the lower hydrocarbons right.

And the diluents right and diluents it can be inert, it can be reactive Diluents right that also effects and people have found out that this carbon dioxide decreases the soot formation when you dilute. But however, if we increase the helium in the as a diluents, helium gas in the air or in the fuel then it is increasing. So, of course, those things are to be looked at why it is so, but if you the soot particle size and then distribution or the this thing will depend on the turbulence level. And particularly one has to look at that whether the turbulence time is higher or the chemical time is higher you know that kind of this thing versus we will have to look at it. And it has been found out that when the inlet temperature is increased particularly for the fuel or the then you find that this the soot generation being decreased soot generation decreases with increase in inlet temperature of the fuel and also oxidizer.

And when we increase the pressure the soot level are the soot formations increases. So, that is the thing people have found out and that is not very general, but at least for the diffusion flame people have jet diffusion flame people have found it. So, one can think of. So, what till now we have basically looked at the jet diffusion flame and we will be discussing about now the going moving into the liquid will combustion because, till now we have looked at basically the gaseous fuel combustion right. And today we will be initiating discussion on the liquid fuel combustion.

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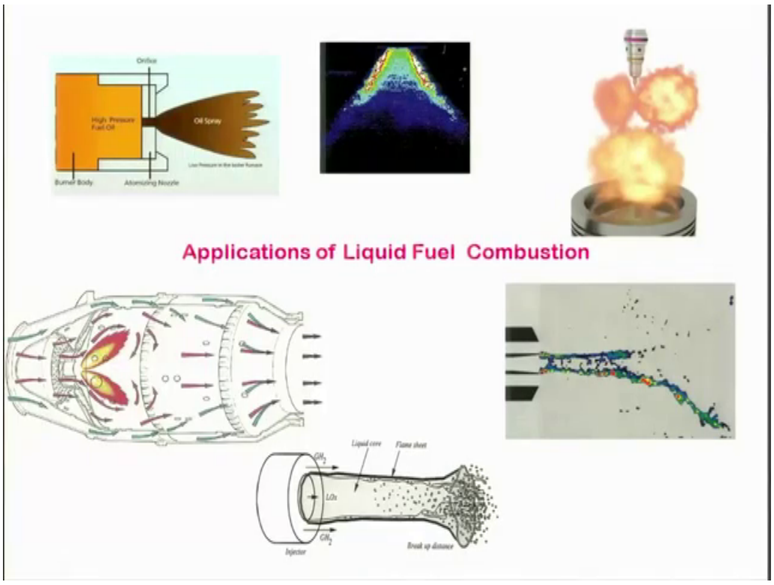

Applications of Liquid Fuel Combustion

So, if you look at the applications of liquid fuel combustion it is quite a bit and if you consider that basically the aerospace application this is the gas turbine engine. And this is of course, rocket engines I have shown here it is a liquid oxygen and then gaseous hydrogen. And of course, this is your diesel engine this is a spray which is coming diesel engine right C I engine compression ignition engine right and this is a furnace.

Where you are using high pressure you know fuel oils to use and this is the oil spray right is being generated and this and there are several application where you will be using the liquid fuel and question arises. Why we will go for the liquid fuel?

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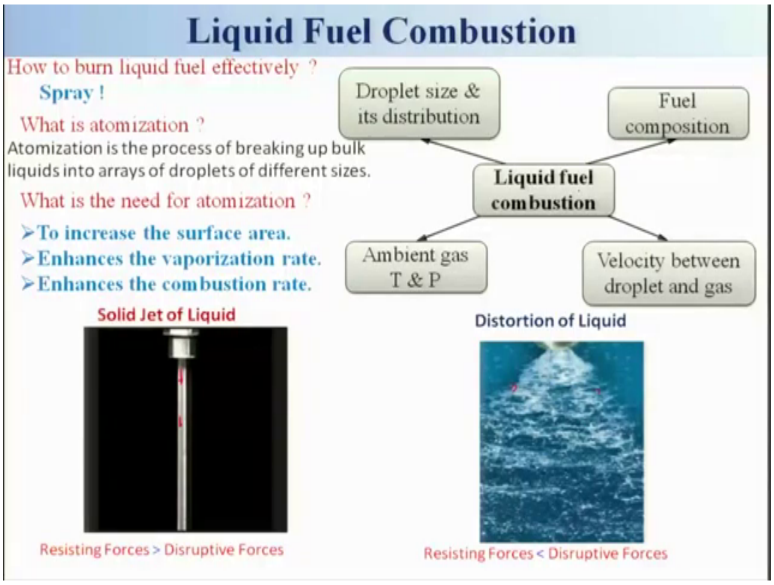

Liquid Fuel Combustion

How to burn liquid fuel effectively ?

Spray !

What is atomization ?

Atomization is the process of breaking up bulk liquids into arrays of droplets of different sizes.

What is the need for atomization ?

- To increase the surface area.
- Enhances the vaporization rate.
- Enhances the combustion rate.

Liquid fuel combustion

Droplet size & its distribution

Fuel composition

Ambient gas T & P

Velocity between droplet and gas

Solid Jet of Liquid

Resisting Forces > Disruptive Forces

Distortion of Liquid

Resisting Forces < Disruptive Forces

And how to burn the liquid fuel effectively is one question. As I told earlier the liquid fuel we need to go for it for transportation and the energy density of the liquid fuel is much higher as compared to the gaseous fuel right and storage is easier for the liquid fuel and also safety other issues are there and, but how to burn the liquid fuel? Is the one question because if I take a pan and do that it will be not serve our purpose. Why? Because that the limitation of the pan size will tell us how much is being burned and how we will control it right that is another question. So, for that what we need to do we will have to basically use the spray that means, you will have to convert the liquid bulk liquid into array of droplets. And that process we call atomization.

So, basically atomization is a process of breaking off bulk liquid into arrays of droplet of different sizes right. Of course, there is a some atomizer which can give mono disperse, but generally in practical situation it cannot be used right, but generally poly disperse droplets are being formed. And a question might be arises in your mind why we will go for that? Right because of fact that this we will go for smaller droplets also or should we go for a larger droplets?

Student: Smaller.

Smaller, but there will be a problem. If you go for two small droplets then what will happen? It will be a leading to a pre mixing of the combustion. And pre mixing means it will be basically subjected to the combustion instabilities and of course, that depends on situation, but generally; so, whereas, the diffusion flame will be less prone to the combustion instability and other things. So, generally on an average that is certain range of droplets which will be used for the design of this thing. So, then what is the requirement for the atomization is basically we need to increase the surface area of the fuel droplets. For example, if I take something around let us say 1 centimeter droplets and I will convert into 1 mm right droplets. Let us say just further then what will happen? That surface area will be increasing very largely because it goes by you know like surface area which goes by the square. Whereas, the mass of the fuel consumed goes by the cube, isn't it?

So, therefore, the surface area will be enhanced very much when you go for an enhancing the vaporization rate because, in liquid combustion basically what has to be done the liquid has to evaporated and then it will be evaporated into the gaseous well. And then it will be come in contact with the oxidizer mixed well and then combustion will taking place. And as a result the vaporization rate will be higher.

So, it will be enhancing the combustion rate. So, that is the reason why we need to go for atomization. Let us see that how we can do that for example, I can pass through an orifice certain liquid and this is liquid let us say it is passing through, this is an orifice the you know it is coming over. And, it is coming as a very nice cube kind of things or a you know solid kind of a jet is coming.

But is it atomize? Now, why it is not atomize? But however, if I will increase the I will use the same orifice, but I will increase the pressure right. That means, if I will increase pressure for the same orifice and same downstream pressure then what will happen? Flow rate will be higher flow rate will be higher means the velocity will be higher right then what will happen? It will be the converted into a very a kind of a spray right.

Now, why it is happening because, here the liquid is basically thin down and it is the ligaments are being formed and then it will be separated out and then it will be converted into the secondary atomization, primary atomize all those things will be taking place. And you will get a very nice distribution of the droplet size, but why it is happening? Because of fact that when it is coming this liquid in the solid jet of the liquid there is a pressure force which is coming or you can say the momentum force that is making the fluid to move right. And there will be also some resistance which is coming right.

If that is with what is the resistance that is the surface tension force which will be making the fluid to adhere togetherness it will be it will be together right. If you are giving more force for to disintegrate because, then only it will possible that means, there will be what we call the resisting forces and there will be disruptive forces. Disruptive forces in this case is less in case solid as compared to the resisting force resistant is the surface tension right.

So, therefore, you cannot really make this liquid jet to disintegrate. Atomization is basically disintegration of the liquid into the droplets. So, therefore, basically, but when it is increasing the pressure what happening the momentum will be higher and the surface tension force will be overcome by the increase in momentum, as a result you know it will be disintegrated. And that is true for us also right always we are subjected to which force one is the disruptive forces other is restoring forces or the resisting forces.

So, that depends upon whether we will make or break you know. Now here our interest is to break the liquid bond of the liquid coalescence kind of things is not really chemical bond it is a you can say physically kind of thing. So, therefore, I will have to apply the more forces than what it could resist.

Let us say if I want to take a you know instead of water or the fuel I will take some thick fluid, it is very difficult to atomize it isn’t it because of that. And, now the liquid fuel will be a combustion will be dependent on the droplet size and its distribution. It will be dependent on the type of fuel what you are using, whether it will be viscous fluid whether it is a what kind of fluid it is having right that also. And, with an ambient gas and temperature of the you know combustors it will be it will be dependent on the velocity between the droplet of gas because, it will be moving. And, keep in mind that this liquid combustion will be dependent on also the extend of mixing and the turbulence level and also the various complex zones what will be there for flame stabilization.

So, it is quite complex in nature. So, with this I will stop over. We will be looking at detail about this thing in the next lecture right ok.

Thank you very much.