Combustion in Air Breathing Aero Engines

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Lecture - 11
Oxidation Mechanism of Fuels IV

Welcome back.

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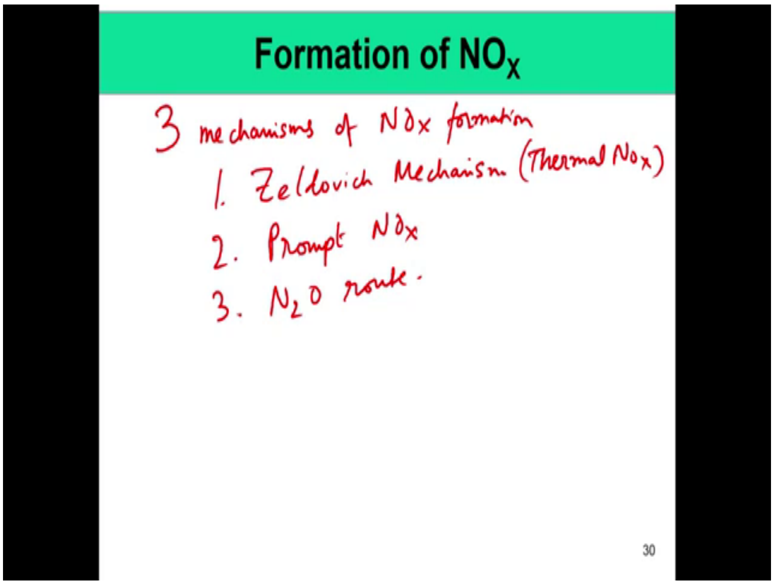

Formation of NO_X

3 mechanisms of NOx formation

1. Zeldovich Mechanism (Thermal Nox)
2. Prompt NOx
3. N_2O route.

Now we will go to the formation of NO X. As we discussed of course, we need to understand ignition delay, but also because that is very very critical in determining whether in a given combustor you will have reactions or not at all whether that given combustor that you have designed whether there is sufficient flow residents time scale for your reaction to happen. Of course, your flow resident’s time scale has to be much bigger than the chemical time scales and the chemical time scale is characterized by the ignition delay time scale of course, you have to guarantee that.

So, it is important to understand where does the ignition delay come from and where is your initiation and plain branching and heat release reaction come from, but at the same time you have to design a combustor of an aero engine in such a way that it produces very little emission in terms of the there is very little emission of pollutants. And one of the biggest pollutant is NO X which is NO and NO 2 which is represented in general by NO X x y is equal to one or x is equal to 2 and also there is nitrous oxide in 2O.

Now these are very bad because it creates smog and it is really very unhealthy and we need to understand the reactions mechanisms that give rise to this.

Now, before we go into this there are essentially 3; 3 mechanisms there are essentially 3 mechanisms of NO X formation one is called the Zel'dovich mechanism or the formation of thermal NO X. The second is the prompt NO X and the third is the nitrous N2O route. So, using these 3 we can describe essentially the formation of NO X in a very comprehensive manner.

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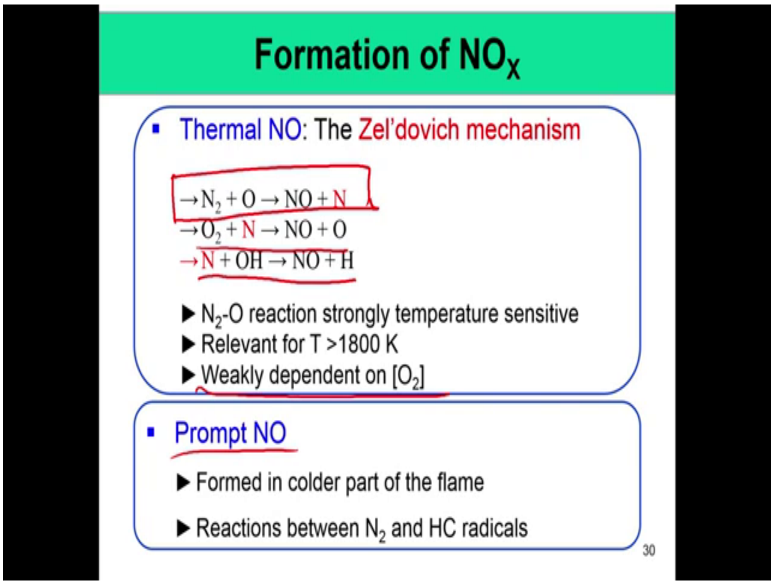

Formation of NO_X

- Thermal NO: The Zel'dovich mechanism

$$\rightarrow N_2 + O \rightarrow NO + N$$
$$\rightarrow O_2 + N \rightarrow NO + O$$
$$\rightarrow N + OH \rightarrow NO + H$$

  - ▶ N_2-O reaction strongly temperature sensitive
  - ▶ Relevant for T >1800 K
  - ▶ Weakly dependent on $[O_2]$

- Prompt NO
  - ▶ Formed in colder part of the flame
  - ▶ Reactions between N_2 and HC radicals

So, what is the first route which is the most important as discovered result are which what is thermal NO X this is called it is obtained by the Zel'dovich mechanism. So, what it says is that the first the most important step which is the first step is when N 2 is attacked by an oxygen atom and it forms NO and NN atom. Now this is the most important thing and then the N atom can react with oxygen to form NO and O and then this N and o H can essentially form NO and H.

So, with the first reaction is a most important reaction where N2Oreaction is strongly temperature sensitive and it is also the reactivity mechanism and it is very difficult to break the N N bond and the N N bond can be broken by an oxygen only at very high temperatures and as a result this mechanism is this; this path is important only are very high temperature of 1800 Kelvin and it is this the thermal NO X is mainly the product NO X that is formed in the product.

But then it was found that end of course, you see that there is no much dependence of oxygen because it depends on the oxygen radical as such, but then it was found that that NO X is also formed in colder part of the flame and it does not need always high temperature to be formed and that leads to the discovery of this prompt NO X mechanism by Fennimore and this reaction between essentially it is a reaction between nitrogen and hydrocarbon radicals.

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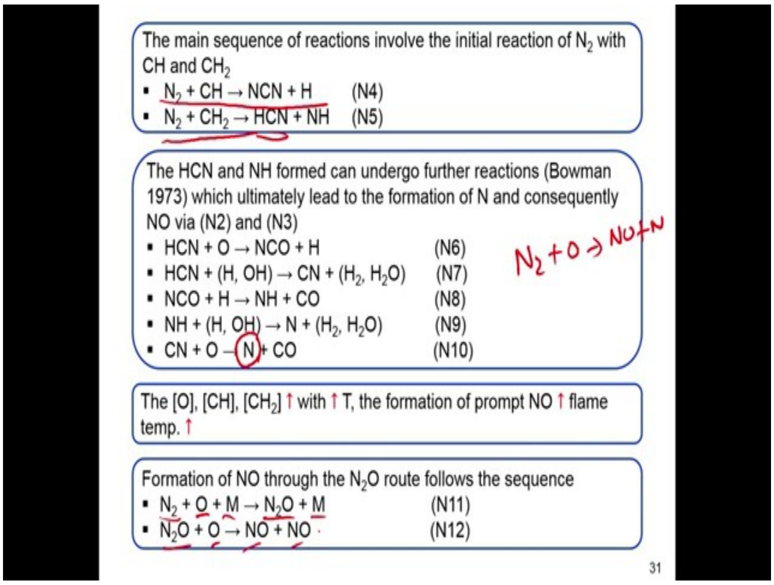

The main sequence of reactions involve the initial reaction of N_2 with CH and CH_2

- $N_2 + CH \rightarrow NCN + H$ (N4)
- $N_2 + CH_2 \rightarrow HCN + NH$ (N5)

The HCN and NH formed can undergo further reactions (Bowman 1973) which ultimately lead to the formation of N and consequently NO via (N2) and (N3)

- $HCN + O \rightarrow NCO + H$ (N6)
- $HCN + (H, OH) \rightarrow CN + (H_2, H_2O)$ (N7)
- $NCO + H \rightarrow NH + CO$ (N8)
- $NH + (H, OH) \rightarrow N + (H_2, H_2O)$ (N9)
- $CN + O \rightarrow N + CO$ (N10)

$N_2 + O \rightarrow NO + N$

The [O], [CH], [CH_2] ↑ with ↑ T, the formation of prompt NO ↑ flame temp. ↑

Formation of NO through the N_2O route follows the sequence

- $N_2 + O + M \rightarrow N_2O + M$ (N11)
- $N_2O + O \rightarrow NO + NO$ (N12)

And its follows this that N 2 essentially reacts with C H to form this NCN molecule and H atom and then it goes through this NCN essentially goes through a different kind of NCN then essentially also this N2N CH2 also confirms HCN N and H and this HCN H and H thus can formed can go through different kind of steps it can be attacked by oxygen, but the most important thing is that all this lead to the formation of N.

Why the formation of N is important because once N is formed you can basically it reacts can react with oxygen to form NO plus O or it can react with oxygen OH to form NO plus OH. So, the formation of N is the most challenging part it can either happen through the prompt NO X mechanism or it can happen through the thermal NO X mechanism where N 2 the thermal NO X. If you remember there is N 2 plus O goes to N 2 plus O goes to a NO plus [noise], yes. So, N 2 plus O essentially goes to NO plus N. So, this was the thermal NO X mechanism that we just discussed.

Now, also you see that these also this prompt NO X mechanism is also promoted with increase in temperature and also it needs the presence of the hydrocarbon molecules actually now the N2O root that we discussed is essentially this is the third body reaction 3 body reaction where N 2 plus oxygen atom can react after being attacked by or can be or a third body also comes in and this N2O is formed and this N2O react with NO to form 2 molecules of NO. So, this is the other mechanism by which this is formed.

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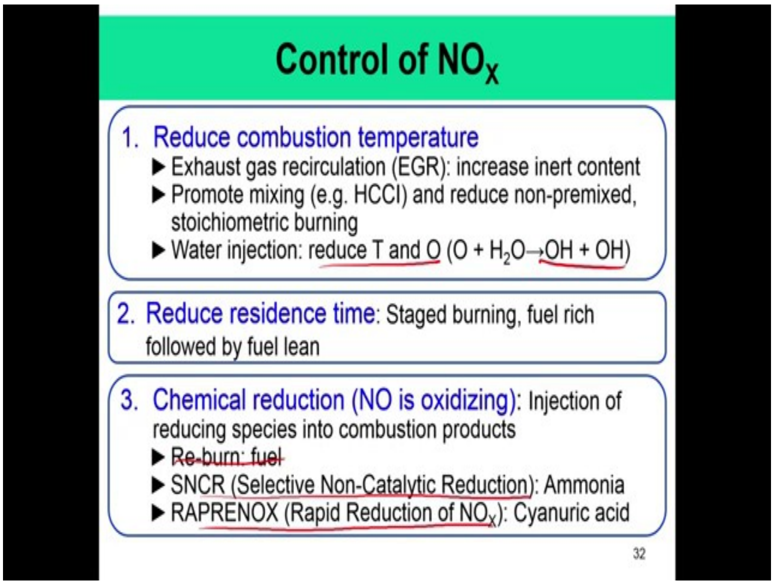

Control of NO_X

1. Reduce combustion temperature
   - Exhaust gas recirculation (EGR): increase inert content
   - Promote mixing (e.g. HCCI) and reduce non-premixed, stoichiometric burning
   - Water injection: reduce T and O ($O + H_2O \rightarrow OH + OH$)
2. Reduce residence time: Staged burning, fuel rich followed by fuel lean
3. Chemical reduction (NO is oxidizing): Injection of reducing species into combustion products
   - ~~Re-burn: fuel~~
   - SNCR (Selective Non-Catalytic Reduction): Ammonia
   - RAPRENOX (Rapid Reduction of NO_X): Cyanuric acid

Now the control of N, I will not go into this there can be different methods by which NO can be controlled it can be done by exhaust gas recirculation and it can be done to promote mixing as in HCCI where of course, we can go to a premixed steroid flame mode as we will see that when a temperature can be reduced at least then the thermal NO X can be reduced. And then we can use the water injection because the water can this they reduce temperature and produce o atoms and the o atom can be taken into form or which can which is essentially this o atom that is present in the in this reactions mechanisms that is formed essentially goes and attacks the N 2 to form the thermal NO X.

So, if you can take away this o atom by reaction with water to from 2OH you basically cut of this thermal NO X mechanism. And also you can do stage burning fuel which followed by fuel lean and there are different other process by which re burn sensitive catalytic reduction and rapid reduction of NO X etcetera these are the methods by which NO X is reduced.

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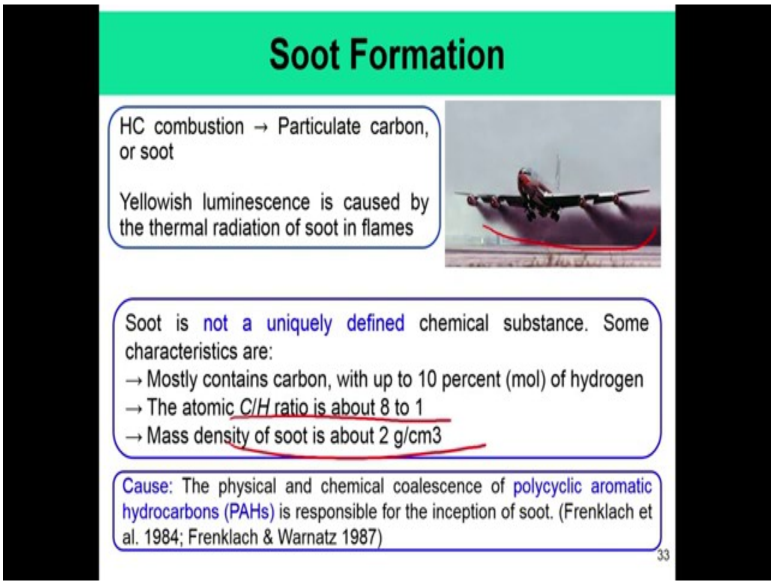

Soot Formation

HC combustion → Particulate carbon, or soot

Yellowish luminescence is caused by the thermal radiation of soot in flames

Soot is not a uniquely defined chemical substance. Some characteristics are:
- → Mostly contains carbon, with up to 10 percent (mol) of hydrogen
- → The atomic C/H ratio is about 8 to 1
- → Mass density of soot is about 2 g/cm3

Cause: The physical and chemical coalescence of polycyclic aromatic hydrocarbons (PAHs) is responsible for the inception of soot. (Frenklach et al. 1984; Frenklach & Warnatz 1987)

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Now, next pollution formation is essentially this soot formation this as you know this hydrocarbon combustion when it happens in rich flames it gives raise to this particulate carbonous soot here you can see that this from this aircraft engine this amount of soot is coming. Of course, nowadays aircraft engines have improved and this amount of soot is rare, but still we need to understand this. There is still substantial soot being formed, because in many aircraft engine combustion happens in non-premix mode and we need to understand the mechanism by which this soot is formed.

So, this yellow luminescence that you see is essentially caused by the thermal reduction of soot in flames and thermal radiation of essentially this soot in flames soot are essentially black bodies and it radiates over a large range of the over huge range of the visible spectrum and it gives out this yellow color that we see now soot is not a uniquely defined chemical substance and its mainly composed of carbon, but it also contains some amount of hydrogen and the atomic C to H ratio is about 8 is to 1 and the mass density of soot about 2 grams per cubic centimeter.

Now why does soot is formed the soot is essentially you will see that the soot is a agglomeration of large number of like carbon small carbon particles and these carbon particles are essentially composed of several thousands of carbon atoms and these carbon atoms can also have different kind of very layered kind of structures which is a; which are and this understanding and the mechanism by which soot formation and the structures of soot is on active research area in combustion currently.

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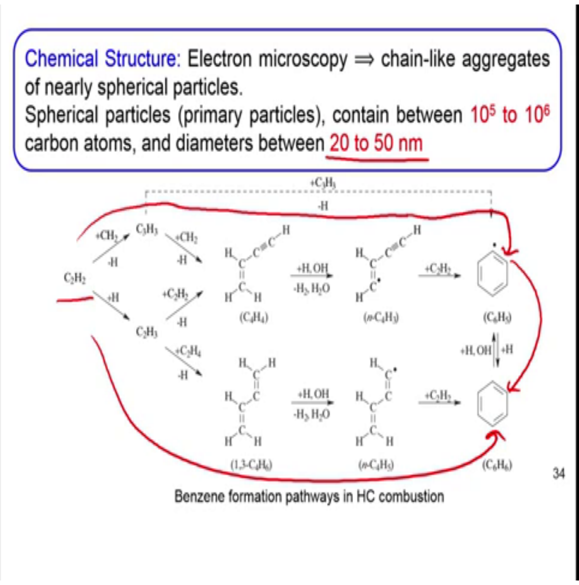

Chemical Structure: Electron microscopy ⇒ chain-like aggregates of nearly spherical particles.
Spherical particles (primary particles), contain between 10^5 to 10^6 carbon atoms, and diameters between 20 to 50 nm

Benzene formation pathways in HC combustion

And as we discussed this chain like aggregates of spherical particles are formed and they contain several 1000s 100-1000s of carbon atoms and diameters of these particles are from 20 to 50 nano meter and the mechanism of soot formation the there are 2 steps essentially or there are 2 it can be subdivided into 2 sets the most important thing is that one of the most important soot precursor is acetylene. So, acetylene essentially you will see that acetylene the C2 H2 can go to different go through all these steps and essentially the it leads to this the formation of this cyclic aromatic compound and then it leads to benzene.

This benzene formation pathway is a very important thing. So, acetylene whenever there is acetylene there are this through all these steps it can go to formation of benzene I will not go into the details of these steps here and then there is also something called precursor to soot which is called poly aromatic hydrocarbons. And so fuel rich combustion has produces acetylene and then acetylene leads to polymerization and formation of these poly aromatic hydrocarbons which is as we discussed.

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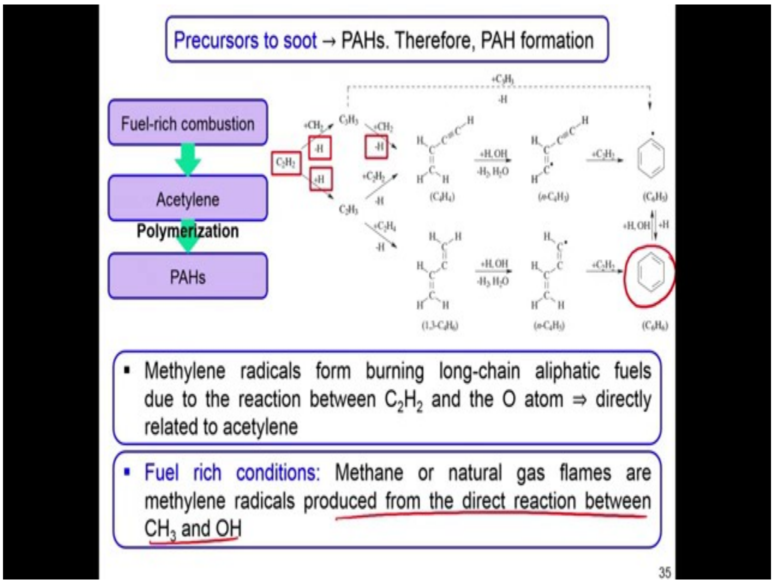

Precursors to soot → PAHs. Therefore, PAH formation

- Methylene radicals form burning long-chain aliphatic fuels due to the reaction between C_2H_2 and the O atom ⇒ directly related to acetylene
- Fuel rich conditions: Methane or natural gas flames are methylene radicals produced from the direct reaction between CH_3 and OH

So, whenever there is acetylene whenever there is fuel rich combustion it essentially leads to formation of acetylene molecules and acetylene molecules leads to this formation of this benzene rings and what happens is that essentially the methylene radicals from burning long chain aliphatic fuels due to reaction between C2H and O atom and directly is related to acetylene and also in fuel rich conditions methane or natural gas flames are methylene radicals produce in direct reaction between CH 3 and OH that is also the thing.

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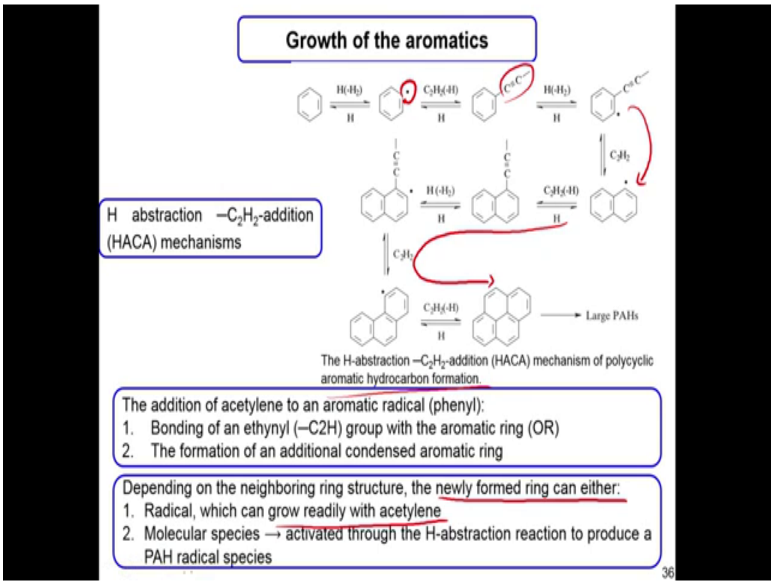

Growth of the aromatics

H abstraction $-C_2H_2$-addition (HACA) mechanisms

The H-abstraction $-C_2H_2$-addition (HACA) mechanism of polycyclic aromatic hydrocarbon formation.

The addition of acetylene to an aromatic radical (phenyl):

1. Bonding of an ethynyl (–C2H) group with the aromatic ring (OR)
2. The formation of an additional condensed aromatic ring

Depending on the neighboring ring structure, the newly formed ring can either:

1. Radical, which can grow readily with acetylene
2. Molecular species → activated through the H-abstraction reaction to produce a PAH radical species

And then how does the aromatic go to form soot’s because the soot is not essentially a benzene ring and that is given by this HACA mechanism which is called hydrogen abstraction by C2 H2 addition the HACA mechanism. So, the thing is that whenever there is. So, we have seen that acetylene leads to the formation of this benzene molecule and then this benzene molecule can be there can be an hydrogen abstraction from this benzene molecule and then we have this free radical and this essentially can have an unpaired electron and this unpaired electron can latch on to an acetylene and now when you know that whenever there is an acetylene there is also a mechanism by which it can form this benzene ring.

So, this benzene ring forms latches on to another benzene ring and so on and so forth, and you can see by this mechanism by this hydrogen abstraction from this benzene ring and then our latching on to that position of this unpaired electron by the acetylene essentially leads to growth of this benzene ring side by side. And that is the hydrogen abstraction by C 2 H by acetylene or the HACA mechanism of formation of poly aromatic formation hydrocarbon formation and these are essentially the soot precursor that is being formed now.

So, this is the thing that that is important in the formation of soot and of course, it can depending on the neighboring ring structure as we see that this newly formed ring can either can go it go readily into acetylene or it can go to or it can be activated through hydrogen abstraction reaction to produce a poly aromatic hydrocarbon radical species.

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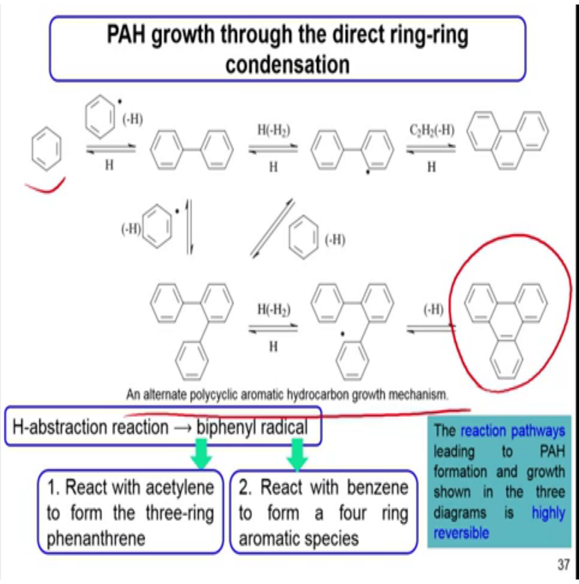

PAH growth through the direct ring-ring condensation

An alternate polycyclic aromatic hydrocarbon growth mechanism.

H-abstraction reaction ⟶ biphenyl radical

1. React with acetylene to form the three-ring phenanthrene

2. React with benzene to form a four ring aromatic species

The reaction pathways leading to PAH formation and growth shown in the three diagrams is highly reversible

So, this is the thing that we talked about right now that if we have a benzene; benzene molecule and the benzene molecule can arise from itself from acetylene and then also it can grow to another path where it can form another alternative poly aromatic hydrocarbon growth formation in which you have this kind of shapes instead of this side by side shapes that we just discussed. So, both of these different structures can be formed by from a benzene ring and then through different variants of the HACA mechanism. So, we will not go into the details in this one.

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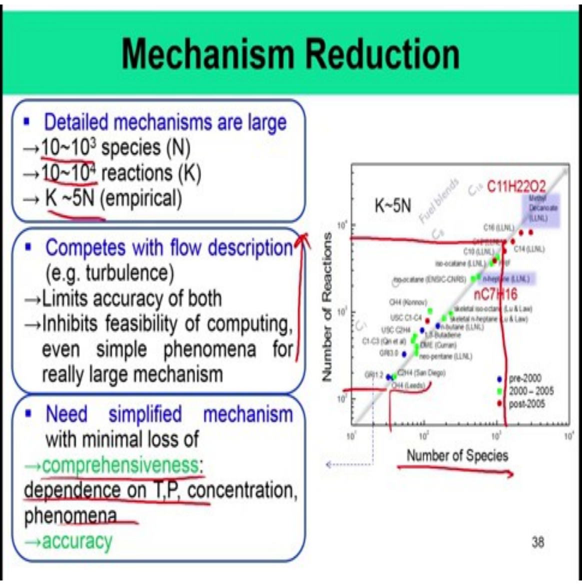

Mechanism Reduction

- Detailed mechanisms are large
  →10~10^3 species (N)
  →10~10^4 reactions (K)
  → K ~5N (empirical)
- Competes with flow description (e.g. turbulence)
  →Limits accuracy of both
  →Inhibits feasibility of computing, even simple phenomena for really large mechanism
- Need simplified mechanism with minimal loss of
  →comprehensiveness: dependence on T,P, concentration, phenomena
  →accuracy

So, now on the on the final topic of this oxidation mechanism of fuels we would like to discuss mechanism reduction now of course, you have seen you have by now understood the importance of detailed reactions. Then we have understood that to predict important quantities like ignition delay etcetera of practical fuels like in dodecane which is an aviation turbine fuel which is essentially representative of an aviation turbine fuel of jet air we need detailed reaction mechanism, because it involves all the different steps you need to understand how this fuel molecule breaks down how it can lead to this chain branching reactions. And then how it can essentially compete with this other molecule other reactions and then when it those reactions can go down and other reactions can go up and these leads to different kinds of complicated things or observations like ignition delay etcetera.

So, to predict this of course, we need detailed mechanisms, but then the problem is that the detailed mechanisms are very large it can range as we can see it can range from 10 to 10000 species and it can range from 10 to 10 to the power 4 reactions that is there can be 10 to 1000 species. For example, the smallest reaction mechanism detailed reaction mechanism that we have seen is that of hydrogen which involves nine reactions nine species 19 reactions and the large ones. For example, in dodecane can involve very very large number of molecules very very large number of species and very very large number of reactions of the order of 1000 species and 10000 reactions and the reactions and species are essentially related by this K to 5N.

And in this diagram if we plot species on the x axis and number of reactions on the y axis you see that that for all things here we see that this is GRI 1.2 and this methane air mechanism that involves about say 20-30 about 30-40 species and more than 120 reactions whereas, this C 60 of this for example, this C 12 which we were discussing this N dodecane that involves about the more about 1000 species and about 9000 reactions.

So, of course, if you want to do a detailed CFD if you want to if you want to solve for or want to predict or want to validate the combustion inside a practical engine one cannot use. So, many species actually in a practical CFD code one cannot use thousand species and one cannot use 9000 reactions if you want to solve for combustion of jet fuels, so, or diaphane which is not even jet fuel, but this representative of the jet fuel which is N dodecane.

So, what you do is that of course, it competes with flow description and it limits the accuracy of both and in this detailed reactions inhibits the feasibility of computing the even for phenomena of a really large even for simple phenomena like computing ignition delay etcetera we have a this is this becomes really too large and even for a simple phenomena like ignition delay and forget about computing for detailed turbulent combustion in a in an actual engine.

So, we need essentially simplified mechanism with minimal loss of comprehensiveness and the dependence of temperature pressure phenomena or concentration phenomena and it should be accurate it should be able to predict things like ignition delay laminar flame speed extension of strain rate we will see what these are essentially, but we know already what is ignition delay it should be able to predict ignition delay at least to a reasonably accuracy and. So, these are the requirements.

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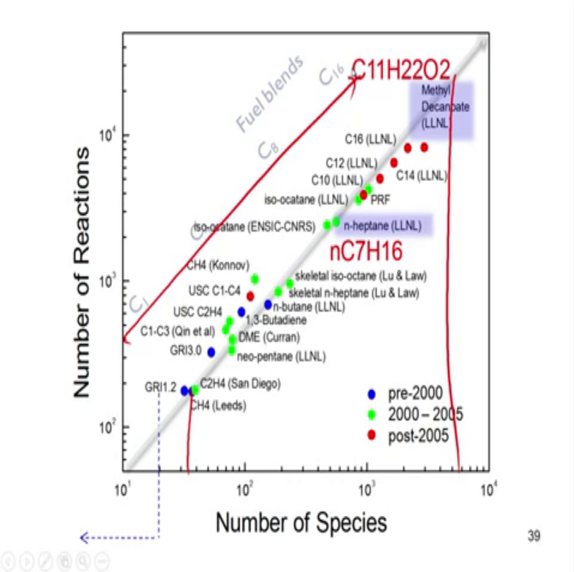

So, this is the once again the detailed this; this diagram proposed by Lu and Tang Sun Lu and Professor C K Lau and you see that once again it can range from this to this very large number of species can be get involved as the complexity of the fuel increases C 8 to C 12 C 16 this sort of things.

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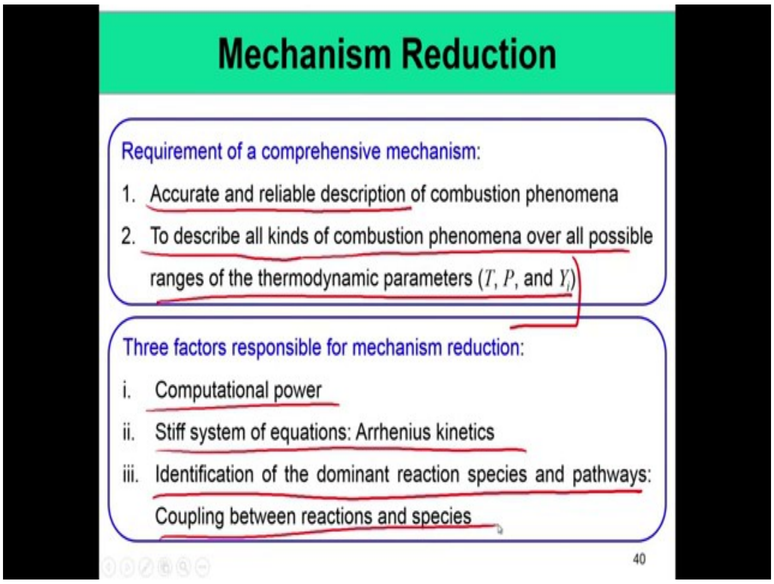

Mechanism Reduction

Requirement of a comprehensive mechanism:

1. Accurate and reliable description of combustion phenomena
2. To describe all kinds of combustion phenomena over all possible ranges of the thermodynamic parameters (T, P, and Y_i)

Three factors responsible for mechanism reduction:

i. Computational power

ii. Stiff system of equations: Arrhenius kinetics

iii. Identification of the dominant reaction species and pathways: Coupling between reactions and species

So, mechanism reduction the requirement of a comprehensive rate mechanism is that it must be accurate and it must be able to reliably describe the combustion phenomena and it has to describe all kinds of combustion phenomena over all possible ranges of thermo dynamic parameters that is t temperature pressure and y species mass reactions the 3 factors that are responsible for mechanism reduction are essentially computational power and stiff system of equations because we have seen all these EA by RT with this reaction rate is different kinds of Es gives us different times skills for reactions. So, that makes this oh, this differential equations of this; this things species quite stiff systems and its complicated and we have to basically identify the dominant species and the pathways and the coupling between the reactants reactions on the species.

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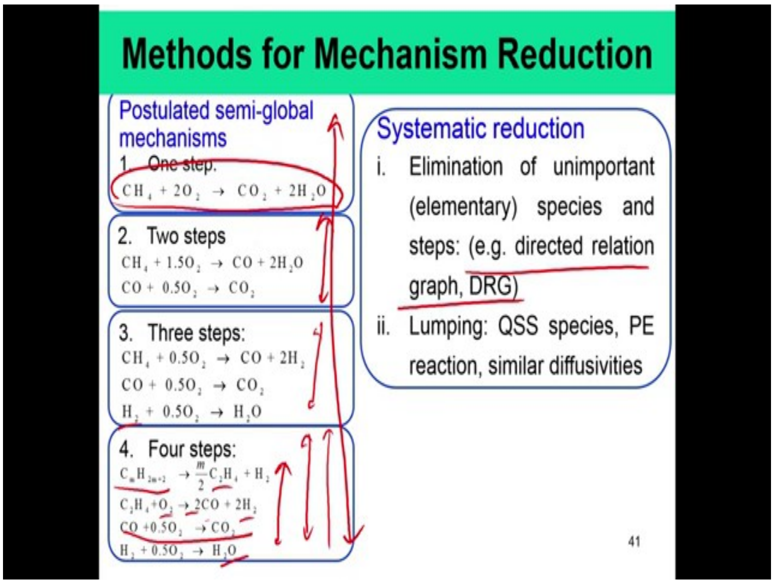

Methods for Mechanism Reduction

Postulated semi-global mechanisms

1. One step.

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

2. Two steps

$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$

$CO + 0.5O_2 \rightarrow CO_2$

3. Three steps:

$CH_4 + 0.5O_2 \rightarrow CO + 2H_2$

$CO + 0.5O_2 \rightarrow CO_2$

$H_2 + 0.5O_2 \rightarrow H_2O$

4. Four steps:

$C_mH_{2m+2} \rightarrow \frac{m}{2}C_2H_4 + H_2$

$C_2H_4 + O_2 \rightarrow 2CO + 2H_2$

$CO + 0.5O_2 \rightarrow CO_2$

$H_2 + 0.5O_2 \rightarrow H_2O$

Systematic reduction

i. Elimination of unimportant (elementary) species and steps: (e.g. directed relation graph, DRG)

ii. Lumping: QSS species, PE reaction, similar diffusivities

Ah now for example, the of course, the most simple reaction one can think of is the one step this is CH4, CO2 plus H2, now of course, you see that we have already known by now that CH4 does not go to CO2 in one step and even CO2 cannot be formed in one step even from CO. So, we need to have a CO in there is the CO oxidation is of course, the most important reactions in one of the most important reactions in hydrocarbon combustions because that is the key step where heat is released.

So, it is natural to introduce CO into the reaction, but of course, these are not actual reactions that happen these are just lumped these are just adding some more details on to a global reactions, by including one step species. So, of course, we can here we include 3 steps where we again and include now hydrogen because hydrogen is also an important step that is formed and then we can have once again an approximate reaction where we have a detailed where complicated alkaline of C m H 2 m and we can have which breaks down into basically ethylene and then this ethylene reacts to with oxygen to form the CO and H 2 and then CO goes to form CO2 and hydrogen as oxidized to form water.

Of course as you know that none of these reactions actually happen like this, but these just adds little more details into a one step reaction mechanism and it considers this important species into border intermediates like C one H two, but of course, to describe this you in details you would need a few thousands of thousands of species and thousands of reactions if say m is large and. So, this is a tradeoff essentially.

So, idea is that that you only consider this was, but this was like done in a ad hoc manner. So, we think that that CO is important we think that H 2 o is important we think that ethylene is important. So, that is why this has been done in an ad hoc manner, but to do it systematically we can consider this we can consider elimination of unimportant species by using this directed relation graph or the DRG and this can be also done by a lumping that is by applying quasi steady state species on this partial equilibrium assumptions which has on also by considering similar diffusivities.

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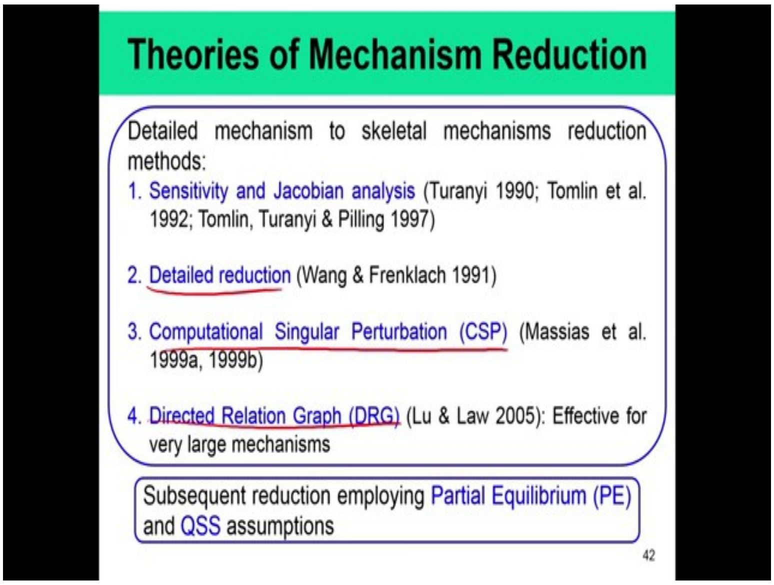

Theories of Mechanism Reduction

Detailed mechanism to skeletal mechanisms reduction methods:

1. Sensitivity and Jacobian analysis (Turanyi 1990; Tomlin et al. 1992; Tomlin, Turanyi & Pilling 1997)
2. Detailed reduction (Wang & Frenklach 1991)
3. Computational Singular Perturbation (CSP) (Massias et al. 1999a, 1999b)
4. Directed Relation Graph (DRG) (Lu & Law 2005): Effective for very large mechanisms

Subsequent reduction employing Partial Equilibrium (PE) and QSS assumptions

So, the theories of mechanism reductions and if you see that they were like detailed mechanism to skeletal mechanism reduction has been has been in people have been active in this area for quite some time this is the main reason because people realize that on one hand if you use one step global reaction mechanism then you get erroneous results you cannot predict many things.

On the other hand, if you want to use the complete detailed reaction mechanism you get you run out of computing power and you run out of memory. So, we people try to find out methods by which detail to skeleton mechanisms can be formed at least by several of these techniques like sensitivity in Jacobean analysis detailed reaction and computation of singular perturbation called CSP and directed relation graph these things.

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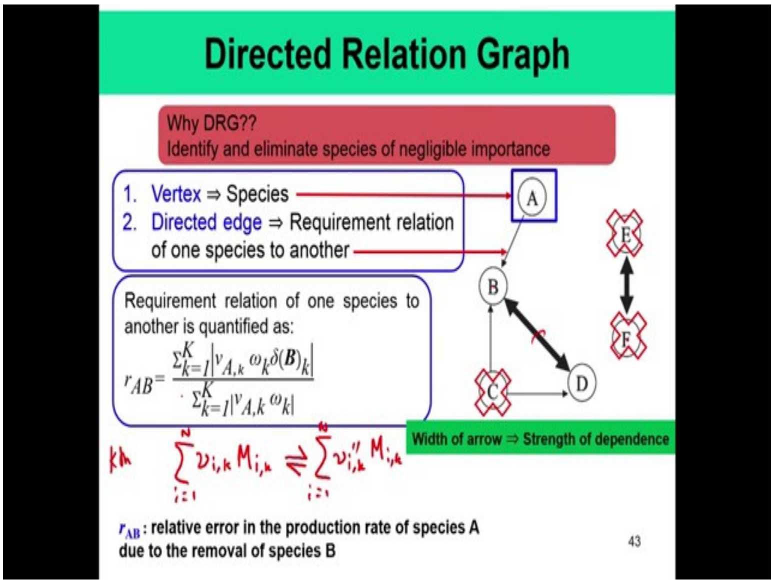

Directed Relation Graph

Why DRG??
Identify and eliminate species of negligible importance

1. Vertex ⇒ Species
2. Directed edge ⇒ Requirement relation of one species to another

Requirement relation of one species to another is quantified as:

$$r_{AB} = \frac{\sum_{k=1}^{K} \left| \nu_{A,k}\, \omega_k \delta(B)_k \right|}{\sum_{k=1}^{K} \left| \nu_{A,k}\, \omega_k \right|}$$

Width of arrow ⇒ Strength of dependence

$$k\text{th} \quad \sum_{i=1}^{N} \nu_{i,k} M_{i,k} \rightleftharpoons \sum_{i=1}^{N} \nu''_{i,k} M_{i,k}$$

r_{AB}: relative error in the production rate of species A due to the removal of species B

So, we will just then subsequently you can you can reduce by implying partial equilibrium assumption quasi study species concepts. So, what is DRG directed relation graphs. So, we think that we consider the reaction a detailed reaction within the species by this by this alphabets A B C D and if this species A and B are reacting we produce we make an edge between them. So, with a directed edge that is A goes to B if it is like that and if it is; if there is if in the reaction between A and B if there is at all any reaction between A and B then we produce an edge.

For example in this reaction mechanism a reacts is a in the reaction somehow A and B are there is some reaction happening between A and B, their case some reaction happening between B and C, C and D and C and B it can be that C is forming into B and A is forming into B and also this there can be some reaction between D and B as the and the as a result they are related here it suggests that B and D are very strongly related, it is a very important reaction, because of certain reasons and which is represented by the width of this arrow of course, there is no connection between a and e and thus as a result there is no arrow between a and e also, but there is e and f are being connected to each other.

So, the idea is that that the it can be quantified by defining this by this relative error parameter which is the summation over k equal to 1 2 k. If you remember the detailed reaction scheme for the k-th reaction it was something like this summation i is equal to one to N for the k-th reaction we could have written like this so, but the A, this was a generalized representation. So, A is the stoichiometric coefficient omega is the reaction rate constant and this parameter will see that how this delta is defined.

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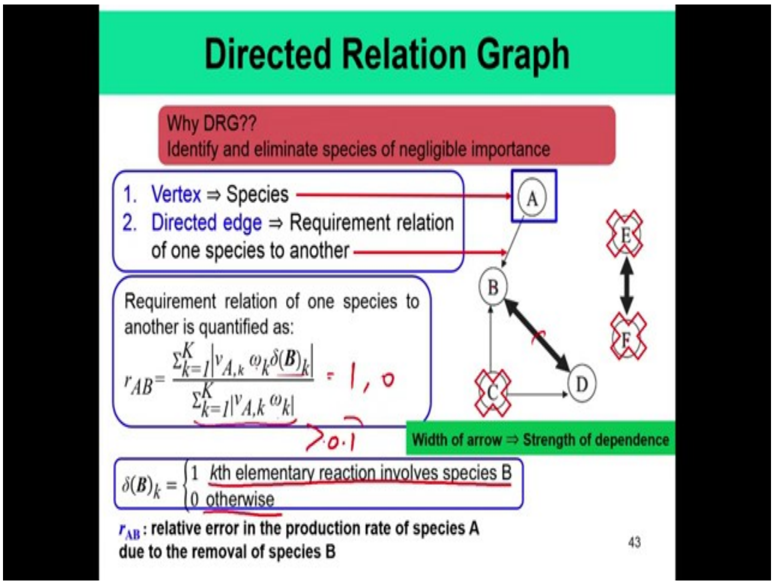

Directed Relation Graph

Why DRG??
Identify and eliminate species of negligible importance

1. Vertex ⇒ Species
2. Directed edge ⇒ Requirement relation of one species to another

Requirement relation of one species to another is quantified as:

$$r_{AB} = \frac{\sum_{k=1}^{K} \left| \nu_{A,k}\, \omega_k \delta(B)_k \right|}{\sum_{k=1}^{K} \left| \nu_{A,k}\, \omega_k \right|} = 1, 0$$

> 0.1

Width of arrow ⇒ Strength of dependence

$$\delta(B)_k = \begin{cases} 1 & k\text{th elementary reaction involves species B} \\ 0 & \text{otherwise} \end{cases}$$

r_{AB}: relative error in the production rate of species A due to the removal of species B

This delta is defined that if this is basically is equal to one if there is A k-th elementary reaction involves species B and it involves 0 otherwise.

So, you see this numerator contains as a summation from k is equal to 1 to k which is k is the reaction number. So, it considers all possible reactions in which A and B can be involved and this stoichiometric coefficient of a in the reaction k it is the reaction rate of k and this is the delta parameter which is defined here and on the denominator we have essentially the stoichiometric coefficient of A and times the reaction rate of k. So, essentially you see that if all involved reaction if all involved of reactions of A involves B then it becomes then this parameter essentially becomes one and this order be is equal to one in the extreme limit on the other hand if none of the reactions involves B then it becomes 0. So, this parameter essentially ranges between 1 and 0 or between 0 and 1.

So, basically this tells you that if you remove the species B that what amount error you will induce. So, if you if this reaction if the reaction between r a between A and B if B is participating in all reactions involving then; then of course, it will introduce a huge error, but if this is not part of participating in very many reactions involving a then the amount of error introduced will be small.

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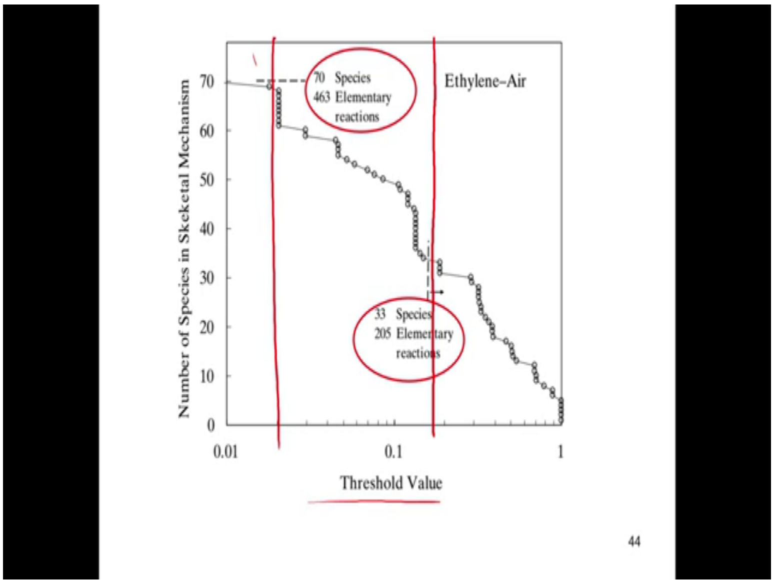

That is what this is saying and using that we can essentially compute this RAV for different parameters and this is how it looks like that this the is the threshold value we can base basically when set a threshold of threshold of RAV that we can say that our we will want to make a reaction mechanism in which we will consider all our species which has threshold which will involve reactions between which has a threshold value of greater than which has a threshold value of greater than point one.

So, and if you see that that if this is essentially the ethylene air reaction mechanism we will see that that this is the how it looks like that and often it happens that this reactions happen in groups. So, for example, if we set here our threshold to be about 0.2, we will see that this will involve a reaction which is 33 species and 205 elementary reactions. On the other hand if you want to set a very low threshold that you want to have very little error you needs about seventy species and 463 elementary reactions. So, this gives us a idea about how to systematically reduce reactions and arrive at smaller reaction mechanisms using this DRG relation and how we can arrive at skeletal mechanism from a fairly complicated and a detailed reaction.

So, that is all for this topic of oxidation mechanism of fuels and we will come back next with on to discuss about transport phenomena. So, all these reactions that we have discussed are basically except for one little bit of discussion where we try to identify the difference between the initiation reactions between a homogeneous system versus that in a that in a flame we have not considered the effect of diffusion, but as you know in practical systems diffusion is very important. And we need to understand; what are the processes that control it and what are the parameters of the parameters that define diffusion or whether the diffusion will happen fast or slow as such like that. So, that is all for now.

Thank you very much.