### Indian Institute of Technology Madras Presents

### NPTEL NATIONAL PROGRAMME ON TECHNOLOGY ENHANCED LEARNING

### Aerospace Propulsion Chemical Equilibrium Analyser -SP 273

#### Lecture 42

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We till now we had discussed a aspects about solid Rockets liquid rockets and hybrid rockets now let us look at how to determine its performance we talked about this that we need to understand equilibrium calculations in order to get to know what is the composition of the gases in the rocket motor and then we need to look at what happens when the when these gases flow through the nozzle remember initially when we discussed about nozzle flow we had said there are two assumptions that are possible one is equilibrium assumption wherein we assume that there is sufficient by time for the reactions to take place.

And because of which if you look at the temperatures that are achieved inside the nozzle because there is a temperature and pressure decrease certain kind of exothermic reactions are favored and you will get a better performance if you have equilibrium conditions and if you have the other condition that is frozen condition that is the composition is frozen at the entry to the nozzle then you will get a slightly inferior performance right.

We can examine those things here with the software called NASA SP 273 earlier it was written in photon language and it was used as such with the input file currently there is a front end available to it and it is called a CA software which you can download from the internet it is freely accessible and if you download this software.

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You will find that it has a manual and it has all the other input files example input files that are there now if you look at the folder in which it is there you will have something known as CAEXC when which if you double-click you will be able to open the software this needs a Java platform to run on okay now if you open this, this software is a more generic software it, it can solve many kinds of problems one is the rocket problem that is of interest to us that is here.

Then in addition to that it can solve the combustion problem that is if you are holding internal energy and volume constant then assign temperature and volume being constant then enthalpy and pressure being constant that is if you are only interested in looking at the combustion chamber of a rocket motor or a gas turbine engine and what are the temperatures that are achieved and other things then you can use this again you have assigned temperature and pressure it can also do the shock tube problems and many other problems.

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Now let us in this case look at only the rocket problem because that is of interest to us so you have to firstly click on this rocket problem now this menu opens up wherein you can define whether you want equilibrium or frozen flow conditions in the nozzle you can click for both because the actual situation will be somewhere in between equilibrium and frozen flow so you have to give the chamber pressures as an input.

So let us say firstly we have to before we go that we have to as I said earlier there are example problems so firstly let us look at the example problem that is there that is example 8 which is stated as a rocket problem okay now here if you look at this is an example problem the initial pressure is set as 53 we can change that to something like 100 bar okay you can input at one time many more pressures 150 bar and 200 bar okay.

You can also have different units in which these can be expressed we will click both the equilibrium and frozen and for the exit you can either define a supersonic area ratio or in terms of pressure ratio so we will define in terms of area supersonic area ratios that is 25 50 75 and lastly we will define something like100 so and finally you have to save this once you say this because this is a liquid propellant problem you have to define the oxidizer to fuel ratio right here are the different ways to give that one as equivalence ratio is also possible then oxidizer to fuel ratio fuel ratio fuel by weight is also possible.

So let us click on the oxidizer to fuel ratios there is one set value that is given here that is the value at which probably you will get the best performance okay let us also click other oh by F

ratios remember we are doing this problem the reactants are if you click on this reactants the same you will get fuel is liquid hydrogen and oxidizer is liquid oxygen forced isometric conditions the 0/ F should be eight so which is why I have clicked eight.

Now because these are already there in the menu so the temperatures automatically come in and the heats of formation are also automatically taken in okay now if you click on this if you click on the name and if you check something is take something as a fuel and if you click on that you can change it from liquid hydrogen to something else also and there are a few options that are available here like methane then there is kerosene JP4, JP 10 all this then there is also RP1 okay.

We will right now stick to what is being selected that is liquid hydrogen and you have liquid oxygen as I said again you can click on this and select any other oxidizer there are various options here that you can look at that is  $H_2O_2$ ,  $H_2O_2$  then RFN, IRNA then  $N_2O^4$  okay so and also a liquid oxygen so we will go with liquid oxygen so both of them are 100% you can define whether you want liquid oxygen as fifty percent some other oxidizer has 50% that is also possible.

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So we will save this and what you have to do is you have to go to this activity and click on the execute see so if you do that it will execute the program and give you an output file in this fashion you can also open this output file as a word the file you can open it as a notepad or Word Pad now if you look at the output it firstly tells you what are the input conditions that you have given the oh by F ratios okay.

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You have chosen equilibrium and frozen and what are the pressures what is the pressure ratios that you looked at and supersonic area ratios what are the reactants and what is the units in which the output file is expressed n so now if you scroll down you will get z okay so if you look at the output file here you will find that firstly the ratios that we have chosen are indicated here then we have said both equilibrium and frozen flow then the various pressures at which we want to run this calculations those are given here.

Then the exit pressure ratios supersonic area ratios and subsonic area ratios and then what are the reactants that we have used and the outputs will be expressed in SI units now if you scroll down this is the place where you will have the results what you can see here is fuel and oxidizers are given the energy the heats of formation are also given here now we will take the case when O/ F is 5.55and the pressure is 100 bar is what we had given now look at what happens to molecular weight this column here is molecular weight the molecular weight is somewhere around 1.8 okay.

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RHO, KG/CU	м	4.4680 0	2.7574 0	4.1849 0	4.1332-2	1.9798-2	1.2926-2	9.5717-3
H, K3/KG		-1026.05	-2225.03	-1242.77	-9563.96	-10337.3	-10726.3	-10976.7
U, K3/KG		-3264.19	-4306-19	-3452.70	-10481.9	-11099.5	-11406.5	-11602.6
6, K3/K6		-63853.9	-61172.8	-63382.2	-36171.8	-32431.5	-38442.7	-29118.6
5, KJ/(KG)(	K)	18.2485	18.2485	18.2485	18.2485	18.2485	18.2485	18.2485
M, (1/n)		12.79	12,505	12.811	13.207	13,207	13,207	13,207
(dLV/dLP)t		-1.01691	-1.01212	-1.01602	-1.00000	-1.00000	-1.00000	-1.00000
(dLV/dLT)p		1.3033	1.2310	1.2904	1.0001	1.0000	1.0000	1.0000
Cp, KJ/(KG)	(K)	7.5133	6.7687	7.3865	3.2154	3.0352	2.9353	2.8696
GAPPAS		1.1495	1.1522	1.1498	1.2435	1.2617	1.2730	1.2810
SOW VEL, M/S	ÆC	1604.0	1548.5	1594.0	1068.4	988.7	930.5	895.4
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So and the temperatures you get a given here this is in the combustion chamber so this is around 3450 almost and this is the throat region as a the flow expands the temperature drops so also the pressure drops okay and further as you go to different area ratios which are given here this is A/80 if you use 68 A/80 then 1.5 8 25 50 75 100 so you can see that both temperatures and pressures keep dropping after the chamber depending on what we have as the area ratio and what this also will give you is specific impulse and vacuum specific impulse.

So you can see that the vacuum specific impulse is always going to be higher than the specific impulse this specific impulse is at sea level we are in the ambient pressure is one atmosphere so you see that at sea level with an area ratio of 68 you will get something like 4384 Newton second per kg it is seen as m/s here which is the same as Newton second per kg so the ISP is that you get are very high if you use a larger area ratio nozzle.

You will get even higher specific impulse that is what you will see here as you change the area ratios the specific impulse also will increase you also can get sea star values which are shown here okay and correspondingly CF values so you just have to multiply c star into CF to get is peace this also gives you as I said earlier that if you look at the exhaust it will have various species so the species that are there are HH,  $H_02$  H2,  $H_2O_2$  OH and O2 and the corresponding mole fractions are given here okay you can see that large fraction is  $H_2O$  okay.

And there is quite a bit of unburned hydrogen right. So this constitutes roughly 95% and the remaining 5% is contributed by the other species so these are the two major species in the

chamber as well as in the exhaust. Now this was with equilibrium right and you can see that if you look at the composition right I can check whether basis at this as some values the frozen flow does not give the correct composition.

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Now take a look at the ISP let us take this last two values will take a look at only the vacuum specific impulse this is roughly 4,600 at 100 area ratio. Now if we do a frozen flow analysis in the nozzle it reduces to 4 4 to 5 at the same conditions of  $A_E$  by 80, so it is very clear that the actual one will probably lie between 4 4 2 5 to 4 6 100 okay. So the actual  $I_{SPs}$  had that we get will be somewhere between this was for 5.5 5 O x f.

Now if you look at O by F of 1 okay the temperatures that you get a very low so therefore the  $I_{SPs}$  that you get are also not very large 3632 and 3700 at area ratio of 100 and vacuum specific impulses 3825 although the molecular weight in this case because the O by F is one right we need a higher over f2 completely burn it O by F of a 8 is required if we use a very low by F as you can see here molecular weight is also very low although temperatures are lower molecular weights are also lower but still as c star is nothing but  $\sqrt{t}$  c by m we finally.

We will get something like 3600 seconds and then if we increase the O/F 22 then the temperatures rise but, so also in the molecular weights and as a consequence you will get to a slightly higher Isp of for 249, then if we go to a no x f of three temperatures go to 2450 and molecular weights, increase to something like 8. So consequently  $I_{SPs}$  go to something like 4469

then further if we increase the O/F to 4 this goes to 4569 it becomes 4475 here in this case temperatures are increasing but molecular weight is also increasing.

So therefore the  $I_{SP}$  change is very small and the best is probably at somewhere around 5.5 55 you get 4603 and 5.5 is where you will get the best Isp this is for liquid propellants.



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The same information is shown here and this graph here which shows on the x-axis chamber pressure and is p on the y-axis there are 2  $I_{SP}$  graphs here one is pH see level which is indicated by this blue line and there is P vacuum which is indicated by this red line which is usually higher both these are for the hydrogen and oxygen system at a know 0 by f of 5.55 and at all these pressures the area ratio of the nozzle is such that the flow is optimally expanded.

Now one can see that as pressure increases the  $I_{SP}$  also increases both the sea level and the vacuum both of them increase.

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Now to understand why it is that we choose an O by f of around 5.55 for the hydrogen oxygen system we have plotted here a chamber temperature c \* and molecular weight molecular weight is in blue color that is this line a chamber temperature is in red that is this line and c \* is shown here in this green line this is it different O/ F and the flow is optimally expanded for a pressure of 70bar, that is the area ratio of the nozzle is chosen such that flow is optimally expanded.

For a pressure of 70 bar that is the area ratio of the nozzle is chosen such that flow is optimally expanded, now if you see at around 5.5 is where chamber temperature is also high molecular weight is also not last large, so you will find that the sea star values are very good now with these Easter values, if you multiply it by the CF which is a function of nozzle area ratio and pressure ratios you will find that you will get a very good is p at around 5.5 which is why most rocket motors which use hydrogen oxygen combination operate around this oxidizer to fuel ratio.

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Now here are compared the hydrogen and oxygen and kerosene in oxygen systems the red line here is the variation of kerosene oxygen with chamber pressure this is  $I_{SP}$  and this is sea level is P we are in with increase in pressure the flow is optimally expanded that is the area ratio is so chosen that at each and every pressure here the flow is optimally expanded one can see that when we change from kerosene to hydrogen as the fuel the  $I_{SP}$  is much higher with hydrogen as the fuel compared to with kerosene as the field.

This is because one the molecular weight of hydrogen is much lower and therefore you will find that the sea star values for hydrogen systems will be larger than what you would get with kerosene and therefore you get a very good specific impulse with hydrogen and oxygen systems.

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And if you look at the sizing of the overall system it depends on the oh by F at which it is operated if you see here oxygen hydrogen and oxygen systems are shown here, this is with different oxidizer to fuel ratio and is p on they-axis the red line indicates kerosene oxygen and the blue line indicates hydrogen and oxygen and the chamber pressure is 70 bar the flow is optimally expanded, so you find that you need a O / f of around 5.5 to get a very good specific impulse whereas with the liquid oxygen and kerosene you need somewhere around 2.5 to get a very good specific impulse.

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Pinf/P	1.0000	1.7719	70.000	86.096	148.66		
P, BAR	70.000	39,505	1.0000	0.81305	0.47085		
Τ, Κ	2826.05	2584.52	1321.67	1270.24	1143.97		
RHD, KG/CU M	7.3872 0	4.5733 0	2.2706-1	1.9209-1	1.2352-1		
H, K3/KG	-2297.31	-2815.24	-5143.75	-5233.11	-5452.62		
U, K3/KG	-3244.89	-3679.87	-5584.16	-5656.38	-5833.81		
G, K3/KG	-30816.9	-28897.3	-18481.5	-18052.0	-16997.2		
5, K3/(KG)(K)	10.0916	10.0916	10.0916	10.0916	10.0916		
M, (1/n)	24.797	24.876	24.952	24.952	24.952		
MW, MOL WT	24,797	24.876	24.952	24.952	24,952		
(dLV/dLP)t	-1.00317	+1.00153	-1.00000	-1.00000	-1.00000		
(dLV/dLT)p	1.0682	1.0353	1.0000	1.0000	1.0000		
Cp, K3/(K6)(K)	2.3818	2.1375	1.7385	1.6178	1.7407		
GAPPIAs	1.1869	1.1992	1.2371	1.2594	1.2368		
SON VEL,M/SEC	1050.5	1017.8	738.1	738.1	686.6		
MACH NUMBER	0.000	1.000	3.232	3.319	3.659		
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CSTAR, M/SEC		1503.9	1503.9	1503.9	1503.9	I	
CF		0.6768	1,5865	1.6112	1.6704		
Ivac, Matte		1866.5	2578.6	2597.8	2663.8		
Isp, (%)		1017.8	2386.0	2423.1	2512.1		
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We will now look at a solid propellant the example 5 problem here deals with a solid propellant but the binder is something different so we will take a look at another example wherein I have looked at htp be as the binder, now if you look at this the 68% ammonium perchlorate 18% aluminum and then 14%  $H_{TTP}$  be as I said if there are if these compounds are not found in the list you have a provision here to indicate a name and then amount and both temperatures and energy and you can also provide a chemical formula here.

I have taken a butadiene formula here C4 H6 which is very good approximation for HT p bh TPB will have and 0 h radical in the end of the chain even if we neglect it does not matter as much to what we are doing, so here what we have to click is for a solid propellant it does not everything is preset in some sense you just have to define what are the percentages and that should automatically take care therefore, we do not have anything clicked in this menu here and if we click at the rocket menu.

We have something like at 70 atmospheres and 70 pressure ratio we can also give something like 10 and 15 area ratios, so we click both equilibrium and frozen flow so now if we look at the output file you have 70 bar as the pressure area ratios and then the various components that is ammonium perchlorate aluminum and  $h_{tp}$  B which is 14%, so now if we look at what happens 70 atmospheres the temperature is very high but because the molecular weight is also quite high you end up getting an I<sub>SP</sub> of around 250 seven seconds.

This is with equilibrium calculations with frozen calculations it will be even lower sometimes this frozen calculation does not work beyond the throat because if you have more of alumina then it does not work for the frozen flow because it then becomes a two-phase problem okay, you are looking at if you look at what are the temperatures this is lower than the aluminum melting point so it will be a two-phase problem and therefore the frozen flow will not be able to solve for it now one can also look at this is with.

If you lower the pressure to something like six bar you notice that this temperatures are also not very high because the if you look at equilibrium pressure is also something that determines, what is the equilibrium composition and therefore the temperatures will depend on what is the pressure, so you will get a lower temperature and correspondingly a lower ISP what this software will not be able to tell you is look at the ISP column with 15 area ratio and with 6 bar right, so the pressures if you are doing this experiment at sea level the exit pressure is very, very low right and in this condition.

You will have probably a normal shot setting in the divergent portion of the nozzle and therefore you will not be able to get this kind of ISPs but unfortunately this software will not be able to tell you that, so one needs to be careful and look at the exit pressures while doing this if you are doing sea level operation you need to be careful about what is the exit pressure and use the Summerfield criterion which is something like one-third of the exit pressure is what it can take without any problem okay.

Now one can also change the remember we said if we make this aluminum is added only to enhance the specific impulse, so let us say we make it 0% and this 86% so ammonium perchlorate and a binder only, so then if you run the 2385 so it has reduced because aluminum content is not there look at the other thing that the temperatures here you get is lower molecular weight is also lower, but in that case the temperature was higher and molecular weight was high higher by it went up to something like 27.

So therefore this was around 3400 and this was 27 therefore you ended up getting a higher specific impulse.

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Now solid propellants we have just now seen how its  $I_{sp}$  varies with the pressure here we plotted a pressure on the x-axis and  $I_{sp}$  on the y-axis and at each and every pressure the flow is optimally expanded that is again the area ratio is, so chosen that the flow is optimally expanded and the red line indicates a non aluminized propellant and the blue line indicates an aluminized propellant.

It is very obvious from this graph that for an aluminized propellant the ISP is always higher because with the aluminum combustion the chamber temperature is always higher and therefore you get a much better Isp compared to a non aluminized propellant and also both of them tend to increase with increase in pressure we will go to liquid hybrid propellants hybrid problems as I said we can look at HT TP be binder and liquid oxygen as oxidizer okay that is what we have selected here liquid oxygen wonder-percent  $H_{TTP}$  be binder 100% okay, now we need to also give O by F ratios, so we can give something like one 2.2 roughly is where you will get the best performance, so if you look at the pressure we have given something like 200 years let us lower at a little 200 and suppose on Ic area ratios ranging from 30 to 60.

Now if we open the output files O / F ratio is ranging from 1 to 3 and we also have 2.2 and fewer less  $H_{TP}$  be oxidizer is liquid oxygen and pressure 100 bar and area ratios we see that at O / F of 1 the temperatures are very low and as a consequence you will get something like to 60 seconds or two to 74 seconds with vacuum is P, if you go to higher oh by Fat to the temperatures increase and also the molecular weights will increase and as a consequence you will get something like 3 27 seconds.

Sea level is P and around 340 seconds vacuum eyes then if we go to something like three then you get these kind of numbers the temperatures has increased but molecular weight is also increased now you can play around with the kind of additives that you would want to add let us say I talked about aluminum hydride as a possible additive that can increase the specific impulse quite a bit so we will select aluminum hydride is already there I just need to put something like 50% aluminum hydride and reduce the binder content.

To something like 50% so overall the binder and the fuel binder and aluminum hydride put together is one 100%, so now if we run this here you see we have added aluminum hydride that is around 50% and binder has been reduced to 50% somewhere around to the temperatures are very high and so also the  $I_{SP}$  is high 341 seconds and vacuum is P is 361 right, and at an O/1 if it is 351 and 367 seconds you see here as O / F is reduced the molecular weight is getting reduced and the temperatures.

Are all sort of smaller but what we are interested in is a combination and therefore we end up getting a better performance at this O by F now if you go to a no x f of 3 the molecular weight has increased to something like 30 and the chamber temperature is 4,000 but the  $I_{SP}$  you will get is lower, so with aluminum hydride it offers you can also change the fraction of aluminum hydride and find out where you will get the best performance what we have probably selected is not the optimal so you can play around with it and find out at what fraction you will get a better performance aluminum hydride is a good.

Additive to add because it can the increase the specific impulse and if you look at the specific impulse with HT PB and locks as I said earlier this is very similar to what you will get with kerosene blocks, but if you want to go beyond that you have to use something like aluminum hydride which will increase the specific impulse even further here there are two hybrid systems that are compared on the x axis.

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You have chamber pressure and on the y axis is P the red line is for aluminum hydride and HTTP be 50% aluminum hydride 50%  $H_{TTP}$  be and liquid oxygen the blue line is for liquid oxygen and HTTP be the 0 by F is two for the blue one and the 0 by F is1.3 for the red line that is aluminum hydride propellant and in all these cases the flow is optimally expanded now if you see here with aluminum hydride being added at the expense of HT PB we do tend to get a very good specific impulse and this tends to increase with sure.

So there is a difference of around 20 seconds in Isp between these two so adding  $\alpha$  aluminum hydride is a very good thing it will help in increasing.

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The  $I_{SP}$  the again we are comparing aluminum hydride propellants with the  $H_{TTP}$  B&O to propellants this is again a hybrid rocket here we plotted with 0 xf and Isp on the y axis this is for a chamber pressure of 70 bar and again the flow is optimally expanded what we see here is another interesting feature the red line is for aluminum hydride and  $H_{TTP}$  be combination and the blue line is for hydrogen H TPB and oxygen system, now if you see here the peak specific impulse is achieved with aluminum hydride propellants at around 1.

Whereas it needs to go to somewhere around 2.2 for HT PB & 0 to what it indicates is that if you use aluminum hydride you will get a much smaller or a much more compact system with density impulse being higher because the 0 by F at which the best specific impulse is achieved is at one usually liquid oxygen which has a density around 1000 140 as lower density compared to the solids and this here has a density around 1200 2300, so therefore you will get a very good density impulse and this is this makes the system is smaller.

So you can as I said play around with this and try and generate your own numbers one way to check whether you have done something correctly is look at literature if you do a solid propellant what are the ISPs to get and then find out if you redo the same will you get the same, so and then you can you get the confidence you can play around with this and look for other additives and things like that okay we will stop here thank you very much.

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