Concepts of Thermodynamics Prof. Aditya Bandopadhyay Department of Mechanical Engineering Indian Institute of Technology, Kharagpur

Lecture – 07 Use of Computer as Means of Learning Thermodynamics

Hello everyone and welcome to this lecture, in which we will see how with the aid of a computer, we can make calculations of thermodynamics. So, for this purpose we will make use of a software called as EES.

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This is the abbreviation of Engineering Equation Solver. So, you go to www dot f chart dot com slash ees and then you have a page, where you can download a demo version of it.

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A demo version of it has various limitations, but for our purpose I mean for what we intend to do, we intend to make use of various properties and do some calculations. The idea behind EES is to not have black box, it does not solve everything for you. The thing is you have to tell what it needs to do, you have to tell what properties it needs to fetch and then it will look up the database, the database typically one would read from a book.

You have a table sub-data corresponding to this temperature, this pressure, this energy and all this things. So, instead of doing that manually the computer does the look up does the look up for you and then what you do on a calculator can be done on this software.

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I mean this software has various other, I mean abilities it can do single variable optimization, it can solve ODEs, it can do non-linear equations and so on. It is very robust and flexible software.

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But the demo version we will use primarily for this academic purpose for learning, various concepts of thermodynamics. So, when we go to the demo we even click on the demo its inside downloads it opens this page, where you have to do a quick registration for EES on windows.

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So, we put in the details and you use it for educational purpose, because if you want to use for professional purpose, you need to buy the software.

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And you click on I am not a robot and then the whole AI business starts. Nowadays it is a big thing so, with fire hydrants good I am not a robot and then you submit. So, download a working demo click here to download. So, let us click over there. So, then we save it we on our desktop I mean we can save it wherever, then we go to the folder and when we install the software that is as easy as this.

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You can change the path of your installation, as you like it is a very flexible software and then it opens up this screen; so, demonstration version for evaluation purposes.

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rajor difference between EES and existing equation solving programs in the many built in mathematical and thermophysical property functions which EES proiders. For example, the sharen tables are implemented such that any		
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15 provides the capability to do parametric studies. Selected variables can be included in a spreadoheet like table. The user determines which variables are independent by entering their values in the table cells. EES will solve		
Lable to determine the values of all dependent variables. A plotting option is provided to display the relationship between any two variables in the table. The plot option also provides properly diagrams (such as pressure enthalpy)		
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E5 offers the advantages of a simple set of intuitive commands with which a nonice can quickly learn to use for solving numerical problems. The large data havis of thermodynamic and transport properties built into EES are helpful		
soling problems in thermodynamics, field mechanics, and heat transfer. Additional data can be added by the user as functions (written in Pascal, C, FORTRAN, PYTHON or EES) or in a tabular form, which EES will		
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This demonstration version is limited to only 50 equations, but 50 equations as you will see is a lot of equations ok. So, first thing is first let us I mean create a new file. So, this is how the window screen looks like I mean so, they have also given us a small example of x square plus y cube equal to 77. So, let me try to first increase the font, we go to options preferences, font size, let us make it 18 yeah that is more like it.

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So, let us create file new and let us paste this ok. So, the thing is the copy paste cut print these options have been disabled in the demo version of this EES. Of course, the complete version of EES does support all these operations, but as a penalty for the user to use a free software. A free version of the software they have disallowed us to do all these things, but anyway let us see how an equation a non-linear equation can be solved.

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So, let us say we have this equation x square plus y cube equal to 5 and x minus y equal to 2, you have written down the equations in the equation window and then we have to

go to this icon which is solved, calculations completed 2 equations in 1 block. And it shows you that the residual is this, the fact that its showing a residual implies its using some kind of a non-linear solver, and thus the solution obtained is x equal to 2.33 2.233 and y equal to 0.2332 ok.

These two are the solutions for these non-linear coupled equations. So, it does not matter what order you input your variables as, but as long as it has the variable as long as it has the equation it will solve it. So, in the case of thermodynamics, it has various in built functions ok.

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Let us try to do a very simple example let us try to determine the pressure so, the comments. So, because it is a demo version it will not let me save as well the comments can be written in curly braces.

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So, if you run this thing becomes blue if you buy the full version of course, you can save the file. So, we open a comment and then we write the nature of the problem. It is for us to understand the more comments you write the better, it is for others to understand what you are trying to actually do.

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So, the question is determine the pressure for water at 200 degree Celsius, with v equal to 0.4 meter cube per kg. So, in this particular problem we have to find the pressure of water for which the temperature is given and the volume is given.

So, in if you have to do this by means of the manual tables you would go to the table and then first you would have a look at what the properties are at 200 degree Celsius. Is so, one would check if v equal to 0.4 meter cube per kg lies between the specific volume of vapour and liquid.

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Essentially you would check if 0.4 lies between this particular point and this particular point is 0.4 over here, or does it lie somewhere between the vapour and the liquid, if yes then the fluid is in a two phased region ok. If no then we have to check if the volume is larger than this or smaller than this, if it is larger than the saturated vapour volume, then we know that the final solution corresponds to super heated zone, if it is less than that it corresponds to a sub cooled region.

So, in order to do that you have to first look up the saturated tables determine a v equal to 0.4 is actually a saturated property or not. If it is in the super heated zone, you will then make use of the super heated tables and determine then the temperature the pressure, but here in EES you would simply write P is equal to pressure vapour, T equal to 200 and v equal to 0.4 steam, it is not vapour its steam.

So, it gives an answer of 530.4, but what are I mean how do you make sense of anything what is 530 ok. So, in order to do that one has to see what the units are so, you click over here it gives you a window which shows the preferences. So, the unit system is SI units see, the older books and older systems of engineering sometimes they follow English

systems pounds foot and all these things, but we do this. Specific properties is on a mass basis see specific volume is the total volume divided by total mass. So, you can also have specific molar volume, this is the total volume divided by total number of moles. However, if you select that then only it becomes on a molar basis, but now we are working in a mass basis because, that is what we have followed in the theory class. The temperature units it is in Celsius this is the very important step ok, ideal gas equations and all this work in Kelvin, but typically for engineering one works with Celsius. The pressure units are kept as kilo Pascal very important, because typically what the pressures are used you will report them as either kilo Pascal or mega Pascal. Rarely will you use Pascal or bar as a unit sometimes we can use bar also, but usually its kilo Pascal or mega Pascal.

For example the atmospheric pressure is 0.1 mega Pascal or 100 kilo Pascal approximately. So, the energies are also reported in kilo joules and the trigonometric functions are used in degrees, see these are what naturally we write 60 degrees and all this ok. So, Celsius and kilo Pascal are the more important things to be noted right as of this moment.

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So, this output pressure that we obtain over here is in kilo Pascal. So, the answer is: 530 kilo Pascal 530.4 kilo Pascal, but wait so you want to actually observe where this point lies in the PV diagram or the T v diagram. So, instead of writing T as 200 so, 200 was in

degree Celsius that is why we write 200 and not we did not convert the temperature into Kelvin because, we are naturally using the units as degree Celsius. Even in the tables of the book you will use degree Celsius as the unit.

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So, let us write this as T 1 and let us write this as v 1, where we have declared everything as an array now ok. P 1 is the first element of the P array, T 1 is the first element of the T array v 1 is the first element of the v array actually to avoid any confusion, let us write this as temp let us write this a vol and let us write this as pres.

See because inside this function so, pressure is the name of the function. This is the name of the keyword. This keyword is what tells that look up the tables of steam, this is the keyword which tells the function pressure that look up the steam table whose temperature I am giving you, that is why T equal to see later on we will see that we can use enthalpy entropy internal energy and all these things. So, that is why you need to tell the computer that which property do you want to use to calculate the pressure.

In this case we will use temperature and volume hence v equal to vol 1. So, let us define temp 2 as 200 and vol 1 as 0.4 after running this we obtain an arrays table where we have the first entry of pressure as 530.4, the first entry of temperature as 200 and the first entry of volume as 0.4, we can now plot this we go to plot we o to new plot window we go to xy plot.

In xy plot suppose we want to plot ok. So, before this we actually need to draw a property plot, because we want to superimpose this particular point on a property plot. So, we go to plots we go to property plots then we have to select what kind of fluid we want. So, we (Refer Time: 15:39) go to water a steam ok, you are working with steam. So, then we want to select the type of plot property plot that we want. So, let us do it in a T v plot, then additional things that you have include lines of ok. So, let us deselect this one now.

So, these are isentropic points isentropic lines these are isobars, in our particular case let us draw 1 particular isobar or let us draw 2 particular isobars, 1 at 500 kilo Pascal and 1 at 400 kilo Pascal, because we already know that the solution is 540 point something. So, let us draw the 2 isobars, it will help us to understand, where the point lies in a better manner ok, we deselect show lines of constant quality as well.

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So, once we press on ok, it will create this particular figure ok. So, on a T v plot this is the isobar corresponding to 400 kilo Pascal and on top of that is the isobar corresponding to 500 kilo Pascal ok. So, volume is in a log scale if you do not do this the plot will look very odd we can change the x axis limits from 10 raise to minus 3 to 1, because we do not really bother about this region. So, let us double click on this we go to y axis oh sorry the x axis and the maximum we call it as 1. So, now, it has rescaled the plot for us.

Similarly, on the y axis let us draw it till 400. So, the minimum is 0 and the maximum is 400 let us say that the minimum is also 100. So, this is how the plot looks like very neat very good. So, this point is 500 kilo Pascal this is 400 kilo Pascal. Now, let us overlay the array points that we had just obtained see we have declared everything inside the array. So now, we can choose these points and plot it on top of this property plot. So, so that we can know exactly where that point lies. So, we go to plot overlay plot and on the x axis we need the volume. So, we say that vol i on the y axis we have temperature temp i and we denote the point as a symbol as a filled square of colour blue there you go.

So, this corresponds to 500 and 40 kilo Pascal it is above the 500 line. So, ideally we should have plotted another line. So, anyway we can do that we can do another plot in which we add, let us add the 540 kilo Pascal line as well and let us add 600 T v, this is the new plot that old plot window is still over here we can get rid of it. On this new plot we quickly readjust the axis. So, the middle line is 540 and then on this plot we can do a plot overlay plot on the x axis, we have the volume on the y axis we have the temperature, we plot it as a blue square and it lies on the isobar.

So, clearly this point that we sort is corresponding 200 degree Celsius and corresponding to a specific volume of 0.4. So, your this temperature this particular temperature is 200 ok. So, it does lie on the 200 degree Celsius line and it corresponds to a volume of 0.4, this is 0.1, 0.2, 0.3, 0.4 it is a log scale this is 0.4. So, this is how we have obtained the coordinate, where that point actually lies and this black solid line is the two phased region anything inside that, anything inside this is the two phased zone and clearly our point lies in the super heated region.

So, the corresponding point is in the super heated region. Now, suppose someone asks me that is all well and good I want to know what is the specific volume of vapour, corresponding to this particular temperature ok.

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So, I write down temp 2 is equal to so, I want to know what is the specific volume we have already discussed we have already discussed that.

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If the pressure is known then if I want to know this I cannot use temperature as the other property, because temperature and pressure inside this region are not independent I can only use the volume and I need to know exactly what the volume is that is what I am seeking at the just obtained pressure. Let us comment this first, because I want to pull up the plot, this was the plot which we had obtained ok.

So, now I want to know that now that I have found the isobar corresponding to this 200 degree Celsius and 0.4 state, I want to know what this particular state is this particular state corresponds to whatever pressure we have just found. Because this line is an isopressure line and I want to know what is this particular volume. And thus I cannot use temperature as a parameter I know what the temp, I know what the pressure is I do not know what the temperature is and I do not know what the volume is.

So, how do we do that we make use of the fact that if it is a vapour, if it is a vapour then the quality has to be 1 ok. Let us first find out the saturation temperature. So, I want to know the temperature of steam corresponding to P equal to pressure 1, this is the value we just found and x equal to 1 alright. Let us see let us run this so, temperature corresponding to this saturation is 154 degree Celsius. So, this particular point is at 154 degree Celsius ok. Now in order to plot this point I also need to plot the volume fine, let us find the volume. So, we need to find the volume of steam. So, volume here refers to specific volume. So, in thermodynamics we do not do absolute volume calculations we do specific volume calculation.

So, it is understood that the function that we have called here corresponds to specific volume and not total volume this is specific volume, volume of steam corresponding to P equal to pressure 1 and x equal to 1. So, naturally we expect that volume to be less than 0.4, because this volume was 0.4 and from the plot we see that this particular volume has to be less than 0.4 let us see it is less than 0.4. In fact, it is 0.3546 and; obviously, pres 2 is naturally equal to pres 1, this is what we have prescribed we want to know the conditions at the same pressure, but at saturation ok.

So, this what we will write. So, these are the points let us try to plot 0.2 so, we go to plot overlay plot now we select on the x axis we have volume on the y axis we have temperature. So, it will plot all the points that it sees over here it has joined by a red line, but I mean it does not matter, actually it is not a process when you join two points usually corresponds to a process. So, thus this point is on by isobar. So, actually we did not plot the exact isobar we plotted the 540 kilo Pascal as our, but the reality in reality the pressure is 530.4 my bad its 530.4 anyway. So, it is slightly below this; obviously, if at a lower pressure it will correspond to a slightly lower point no problem.

So, this is how we have found this point. Now, suppose someone tells you very good, but I want to now find out what is the specific volume of liquid at this point. For this fine we say vol 3 is equal to volume steam P equal to pres 1 and x equal to 0 x equal to 0, because corresponds to pure liquid pres 3 is equal to pres 1, because we are specifying that the volume has to be that the pressure has to be constant temperature. Obviously, will be equal, but just for the completeness temp 3 equal to temperature steam P equal to pres 1 x equal to 0.

So, when we solve this it now leads a much smaller specific volume, because we know that water when it is in liquid density is 10 less to three approximately ok. Depending on temperature of all these things; so, the specific volume will be 1 by density. So, it is order of magnitude 10 raise to minus 3. So, this is 10 raise to minus 3 all these regions are in ten raise to minus 3 ok.

So, logically its everything is fine, then once again we can plot this on the plot. Now if I attempt to find out the volume of such at saturation using the pressure and temperature, it will throw me an error ok. Suppose I want to find out what the volume of this point is I cannot because at this particular point on all these points the temperature and pressure are constant, because all these points correspond to a zone in which there is latent heat of absorption.

So, any increase in temperature will not occur in this zone, at a fixed pressure the temperature will also be fixed during the change of phase. So, I cannot simply obtain a volume. So, let us say vol 4 equal to volume of steam corresponding to P equal to pres 1 and T equal to temp 3 see; obviously, pressure 1 which is this isobar and temp 3, it is corresponding to this particular temperature of the line. Because temp 3 was the temperature of steam and x equal to 0 this; obviously, means that temp 3 is the saturation temperature. Obviously, both the quantities that I am supplying to this function are the saturation quantities and this will throw me an error ok.

It says P is the saturation pressure corresponding to a given temperature properties cannot be determined from this information. So, it throws an error which says that inside this saturation point, you cannot give me pressure and temperature as two independent quantities to find out the rho by d. Obviously, I can then have some other quantity I can choose either temperature and pressure and then the quality, let us write x equal to 0.5.

So, it is half liquid and half vapour half of the mass is liquid half of the mass is vapour, let us see what the specific volume is there you go its 0.1778 it is somewhere over here ok, this point corresponds to 50 percent mass of liquid converted to 50 percent mass of vapour. So, inside the dome what we have seen theoretically that you have to give two independent properties one of which can be temperature or pressure, the other has to be quality, this is how we do the calculations alternately we can also find out the quality ok. Let us say x so, qual 5 is equal to quality steam P equal to pres 1 and let us say v equal to so, now obviously, I have to give the function some specific volume, which lies between these two bounds.

Let us say it is 10 raise to minus 2, we clearly see that 10 raise to minus 2 specific volume inside the dome corresponding to this. So, let us write v equal to 0.01 so, it will give us some quality which is between 0 and 1 and it is; obviously, less than 0.5, because 0.5 lies somewhere over here. So, the quality at 5 is 0.02519 thus even with the help of volume, we were able to find out the quality. So, volume is also the property the specific volume is also the property which we can use inside the superheated dome inside the super-heated dome outside the saturated dome. You can use temperature and pressure no problem, you can use temperature pressure volume any of this, outside the saturated dome there is no use of quality because quality does not exist everything is a vapour.

So; obviously, if you try to call if you try to call quality for a point which is outside it will give you some kind of indication that whatever you have just, let us say pressure equal to pressure 1 and T equal to temp 1. Because, we can this pres 1 and temp 1 corresponding corresponds to this quantity, it is outside the super the saturated dome it is in a super-heated region. And hence, I can give P and T separately let us see what it gives.

It gives us qual 6 equal to 100 so, 100 indicates to the user that whatever you just given does not lie between 0 and 1 it is super-heated 100 does not mean the quality is 100 it is just a number which the software has encoded to indicate to you it is an absurd quantity which is more than one and hence you have to interpret that as super-heated. Similarly if you give something in the sub-cold region; so, we have given this as the condition p equal too plus one which is this pressure and specific qual 10 raise to minus three somewhere over here ok. So, let us see what the quality we obtain it is minus 100

indicating to the user that whatever point you have just given me is in the subcooled liquid is not in the saturated dome.

So, this is how you have to make use of the software, ideally you would look up the tables in the olden days, or if you go even further you would look in the Mollier charts in the Mollier charts you have always information. But, now you can look up all these properties and do some simple calculations by means of a computer. In this case we are using a software EES there are other softwares which make use of other thermodynamic tables; no problem all this data bases have been made by a very renowned (Refer Time: 35:02) very renowned organizations like (Refer Time: 35:04) NASA and all these things. And, it was meant to be used with a computer for very fast calculations for a very accurate calculations usually this hand calculations may not be so accurate.

So, anyway we will throughout this course we will make use of this kind of computer aided means to solve various kinds of problems. So, I suggest you download a demo version of this like, I have shown try to do simple calculations try to compare the calculations against that of a book find out the volumes and all. And, hopefully you will appreciate how simple life becomes. But, one should not forget that whatever we are doing is motivated by our own understanding of thermodynamics, it is not that the computer is doing something for us. We are telling the computer that give me this value, give me that value; the computer is merely a slave for us, it is just a tool which we are using with this note. I will see you next time.

Thanks.