Fluid Inclusion in Minerals: Principles, Methodology, Practice and Application

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Lecture - 37
Computer Software for Fluid Inclusion Data (Contd.)

Welcome to today's lecture. We will continue our discussion on the different types of computer programs packages for use for fluid inclusion work.

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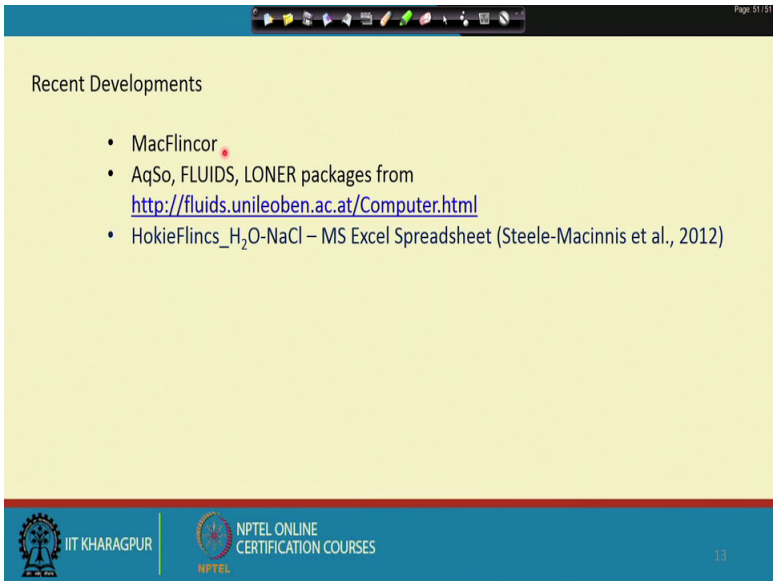

And in the last class, we were discussing about the Flincor package and I think still some people would be using these particular packages of Flincor which was later implemented on a Mac platform and was renamed as MacFlincor and was published and well also distributed. And, it already required a Macintosh operating system for the use of this particular software and they implemented some more features like calculation of the methane mole percent from the graphical or from the graphs that were discussed before, intersection of the carbon dioxide melting temperature and the Persil homogenization of the carbonic face. And but then, MacFlincor also had that limitation that at any point of time, only one particular inclusion data could be processed and then over the past one and half decades, there are lots of computer programs codes on non graphical as well as graphical user interface mode being written and published and the available freely distributed by Ronald J Baecker the university of Leoben and I just been given here this

link for this website. Anyone can visit; anyone can see this website and can get the computer codes that are returned by Ronald Baecker.

So, those computer codes were named in the series of LONER series or the FLUIDS package fluids, AqSo, kind of packages the programs which were return by this author. So, this packages where only is essentially the either exhaustive manner with all available formulations all on different fluid species fluid mixtures, water with electrolytes, with or without the gases only the gases like carbon dioxide, methane, carbon monoxide, water, H 2 S S O 2 so on, hydrogen and so on and so forth. So, all these, so with the over the over the period of time, there has been many workers who have been publishing on the refinement of p v t x relationships on this kind of fluid mixtures either any subsystem of the fluid that I am talking about either a pure carbon dioxide or a carbon dioxide methane or carbon dioxide plus methane plus H 2 S and other sulfurous species or nitrogen argon and so on.

So, the literature on the p v t x relationships in fluids with or without electrolytes so, it also involves the complete range of electrolyte species that we encounter in crustal fluids in natural environment. So, this series of software packages like LONER or FLUIDS or AqSo, they all implemented those formulations and they are written on graph on both graphical user interface as well as non-graphical user interface and anyone will be using like the exactly the way we have seen in the like what was happening in the Flincor package, the user always will be prompted to furnish the data from his raw micro thermometric observations. Often we will you will see that it is prompting for a data to be given in volume percent and such volume percent calculations are made from visual estimation which I have from my experience, which I have said I say that such visual estimation it always give you arrhenius value, but then sometimes they become a better option of the only option there is available if to calculate the volumetric properties. And in addition to what this particular software packages being able to they give the output parameters for any fluid inclusion rock fluid micro thermometric data, they also can be used for computation of the other thermodynamic parameters like fugacity coefficients etcetera from the fluid inclusion data.

So, the participants of this course can always see this particular, can visit this website and see look at the computer codes, ran them and can get a feel of them. I am not using any such demonstration of those particular packages here, anyone can because these days

those computer codes that Ronald J Baecker has developed and his distributing very generously all cross. They will the running on any desktop with either with a presently available windows environment, they comfortable to whatever because there available as executable codes the source codes are not available; the executable codes can be run if it is a the either a Macintosh machine or a windows machine and one can get a feel of the data that that are prompted to be given as input for the raw micro thermometric data. One mention also could been made about this recently released, recently developed excel spreadsheet based computer program which is Hokie Flincs water NaCl which implements the minimum pressure of estimation from a halide dissolution temperature and it is a package complete package on H 2 O Na Cl K Cl from the dissolution temperature of Na Cl and K Cl to give the volumetric property of the fluid in terms of density and this also is available this reference will be given.

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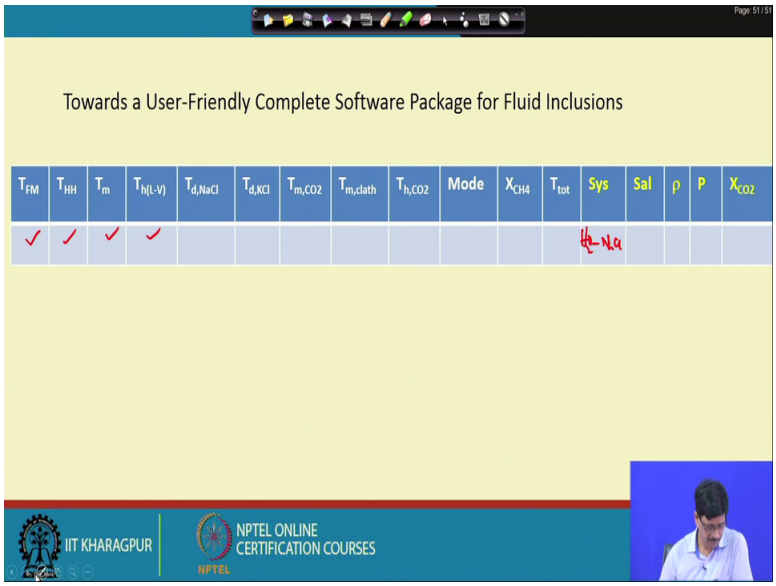

Now, I will I would like to share some of my own ideas and the efforts that I have made in developing computer programs G Y based to computer programmer software for use for fluid inclusion work. Now, this table that have given here is essentially is an is an idea that the first of all the requirement of a fluid inclusions I will talk about a the requirement of a fluid inclusion list presuming that the fluid inclusion list is not an expert in computers or he is not writing his own code, those who can write their own codes or enjoy doing writing their own codes and programs for their own work for the definitely

would always do that, but those who would always like to have something available to use for their for analysis of their fluid inclusion data, it will be more useful for them.

Now, here the parameters T F M is temperature of first melting with corresponds to the you take temperature in a binary or a ternary whatever maybe the system, the temperature of hydro halite melting which sometimes is often even can note observe very if carefully by distinguishing from ice and hydro halite is we discussed. This is the temperature of melting of last ice, temperature of liquid vapor homogenization it will one can always also put another parameter here whether the homogenization was to liquid or vapor, temperature of dissolution of Na Cl, temperature of dissolution of K Cl or again if there is any other face that is there temperature of melting of carbon dioxide, temperature of melting of clathrate, temperature of homogenization of C O 2, then mode or distance C O 2 homogenization, any mole fraction of methane that could be measured by the intersection of the carbon dioxide melting and the homogenization temperature or independently estimated from micro analytical method like Raman spectrometry. And then the temperature of total homogenization for mixed aqueous carbonic inclusion.

Now, these kind of parameters or any other that volcano always have, this is all about this is all that the data that is acquired in a in a routine micro thermometric experiments. The one which are here F M T, H H, T M, T H L V and T D Na Cl, T D K Cl are for aqueous inclusions and T M C O 2, T H C O 2 will be for pure carbonic inclusion with methane with or without methane and then T M C O 2, T M clath rate and temperature of homogenization carbon dioxide and temperature of total homogenization would essentially mean that you are in a aqueous carbonic system. So, the whole of the idea here is that instead of the user specifying or to specifying the program that what system it is inclusion belongs to, the system itself can be very well decided based on what micro thermometric data one has given; for example, if someone is giving at T F M and T H H and T M, T H L V so, this when the when these data are provided, then the system is automatically is coming out to be an H 2 O Na Cl system ; that means, if in a if we think that we are working on and here, we also have to take into consideration that what general the user of a computer a low level user of a computer is essentially familiar with a situation like an Excel spreadsheet where the data can be entered on different feeds. So, if these are the data, these are the columns on which data entered, then the system is automatically is decided that it is H 2 O Na Cl and then it becomes also difficult if to

choose between set of equations rather it should be the set of or the will be formulation which keeps the best result of the most appropriate one within the covering a wider range of the temperature and salinity.

So, then and then depending on if temperature of dissolution of Na Cl ; suppose the data which are entered is temperature in dissolution of Na Cl and temperature of homogenization that also decides that the system is a Na Cl H 2 O system. If it is T D N A C L, T D K C L and T H, so it is a Na Cl K Cl H 2 O system, if there are data which are this actually this logic is absolutely developed here itself.

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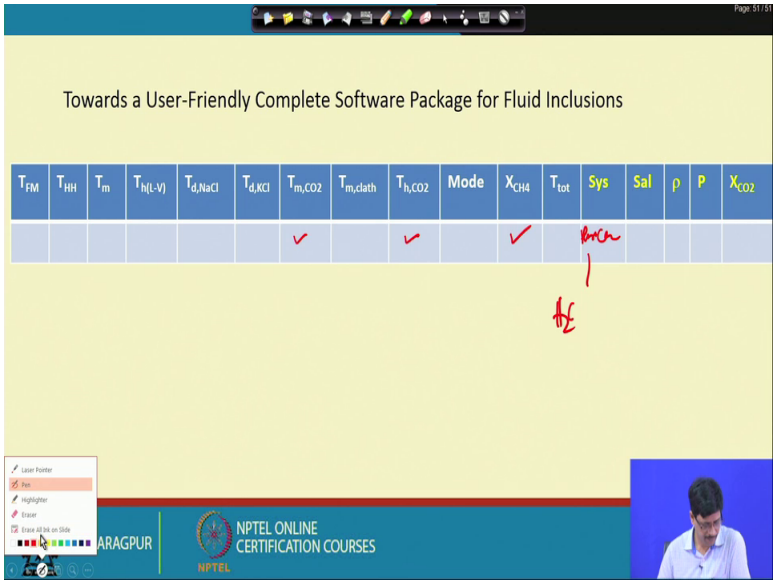

If there is a user which is giving the data for T M C O 2 and T H C O 2 only, then it is definitely is a pure C O 2 and the equation that is going to be used here is the once because the fluid inclusion is always will is an a quandaries to what which equation to use, if is not very familiar with the recent development of the p v t x relationships and which inclusion which formulation to use, this keeps a very; at least it takes away that much of the ration the t yes if the equation the system which chosen and the most appropriate equation to use for a volumetric calculations is also decided.

Similarly, similarly, so if there is T M C O 2, T H C O 2 and also X C H 4 put here as one of the three columns which are filled up then it is an H 2 O sorry, it is a if it is a if it is T H, T M C O 2 and T H C O 2 and X C H 4, then the system is C O 2 C H 4.

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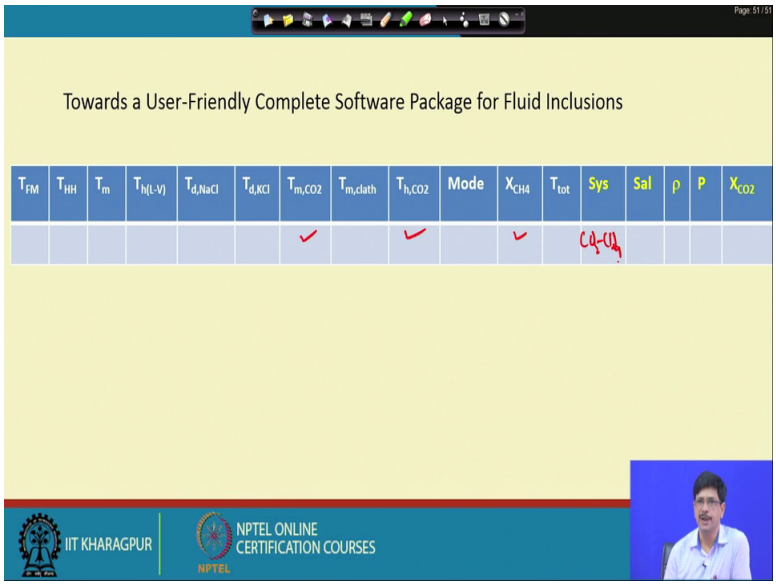

So, likewise this because here it is not a very exhaustive list, but it just for a for the sake of example and it demonstrates that T S if depending on what the data input is giving, the raw micro thermometric data input which is given and the whole idea is give the requirement is that a standard user a fluid inclusion list would during his course of his work would have acquired in for data on all these types of inclusion they could be an aqueous inclusion, aqueous polyphase inclusion, carbonic inclusion, mcaqueous carbonic inclusion and so on.

So, in a in a particular project in a work, there will be a data for all these types of inclusions and it will always be useful if there is one excel spreadsheet which could be where the all the types of data could be entered then all data could be processed at the same time. So, this is a logic behind. So, this could be if that is what is the basic logic of development of any software package it takes into account, the requirement that all the types of data acquired by the by a person who is doing the fluid inclusion micro thermometry are entered at transferred of these days there is some software which are also available interface with the fluid inclusion heating freezing system where the temperature could possibly be recorded. The values of the face changes could be recorded and in such kind of a system which I might myself, I have not work on that the data could be transferred into a excel kind of a spreadsheet here and then one can always go on to process the data. I will just like to give a little bit of a demo on.

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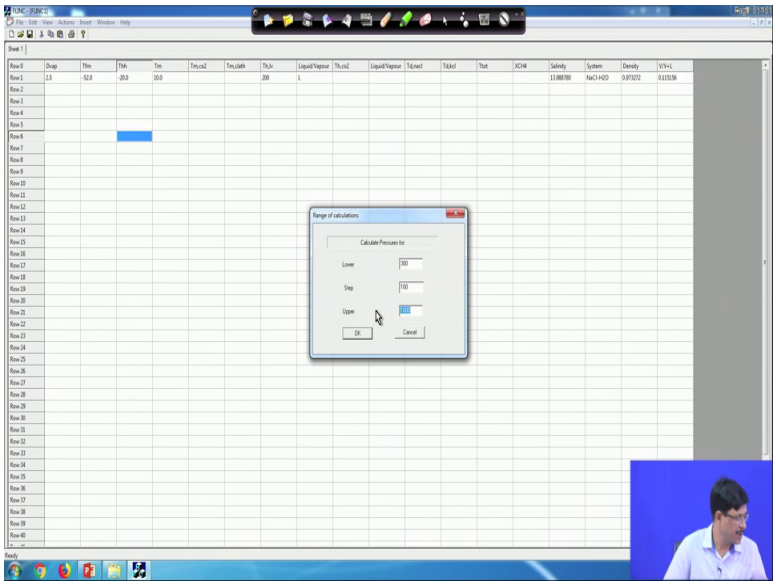

So, this is an example of what this particular packages, but it is near is Flinc was developed on a Microsoft windows based program and using the Microsoft foundation class library. The M F C library which actually after the Microsoft foundation that class library came up, then it became much easier to develop this kind of a user in graphical user interface program, so the packages. So, what is what you could see here that this particular programmers design in generating Excel kind of a sheet. So, what you could see here that this is the d vapor temperature of first melting, temperature of hydro halite melting, temperature of last ice melting, temperature melting of C O 2, temperature of melting of clath rate, temperature of liquid vapor homogenization and then mode to either liquid or vapor temperature of a C O 2 melting and liquid again to liquid or vapor, temperature of dissolution of Na Cl, temperature of dissolution of K Cl T H total. So, these and X C H 4, so what is essential here is that these many number of parameters are the ones which are the input parameters. So, once the input parameters are given, what are the possible output parameters that one would expect? It could be the surface, the salinity, then the system, the density and certain parameter which was at that time also thought to be important is the vapor by vapor plus liquid ratio.

So, say for example, if I just enter a value for a vapor and then diameter of the vapor and then temperature of first melting and the temperature of hydro halite melting I will just give you some example, temperature of last ice melting suppose I put 10.0 and here, as per the formulation the temperature of the depression of the freezing point even though

we know it is value is in negative that the formula has been, the equation has been formulated taking the parameter is positive and then comes the T H liquid vapor and this is 200. Suppose I put 200 degrees and liquid and then here, if I just say click of the mouse a update sheet, then as you could see here that automatically that the system is Na Cl H 2 O that is coming out as the one of the output field.

So, these many output so, we can have many more. This output field are added up or added to the input parameter that are given here and this is the salinity and the density which are calculated. Now, the user who is using this are does not have to decide which equation of state is being used for calculation of density or which equation of equation which is being used for the calculation of the isochore. I say now, this is just one small example and suppose from this particular, so what is the requirement? We take into account the essential requirement for the fluid inclusion list that you would like to generate the plots in terms of the bi variate temperature salinity plot, Isochore and the histogram.

So, suppose this is but this particular data which is been entered for that the isochore needs to be calculated and here, the option of isochore and then this is from the sheet 1 and the row 1 and it gives. So, what exactly it is doing it is using the very basic utilities of whatever is available it could be generated through the Microsoft foundation class library for different types of graphics primitives using the editable boxes that the dropdown menu like the one which is seem seeing here and suppose I put next and as a new chat and then, I could give what is the temperature range in which isochore has to be put.

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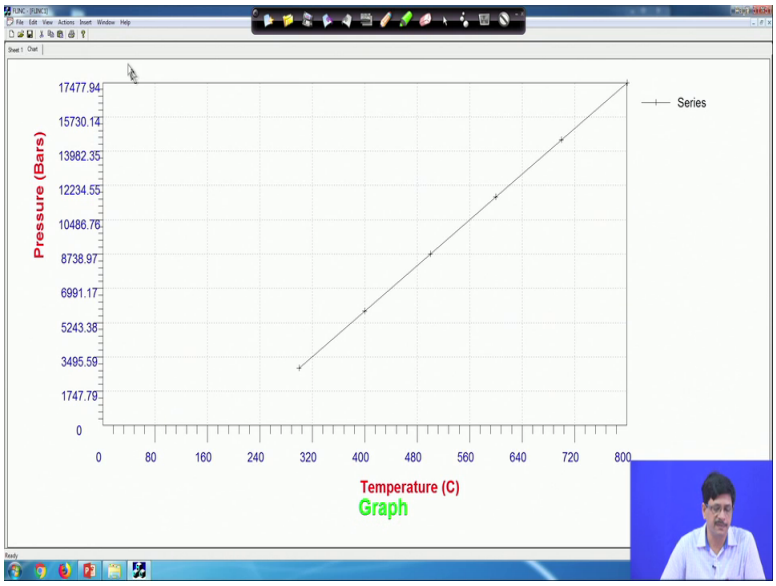

Suppose, I put up to 800 degree Celsius and then say ok, so, the isochore is plotted here. And so, this was this the whole idea full idea of presenting brief is just to give you a feeling that how what logic could possibly we developed in designing or having the software which will be on one particular workspace will be able to give you the entire requirement.

So, I will just give a another demonstration by, so there are all basic utilities which could be incorporated here like for example, I can delete this particular chat if I am not happy with that or I can generate main such graphs and I would just like to ok.

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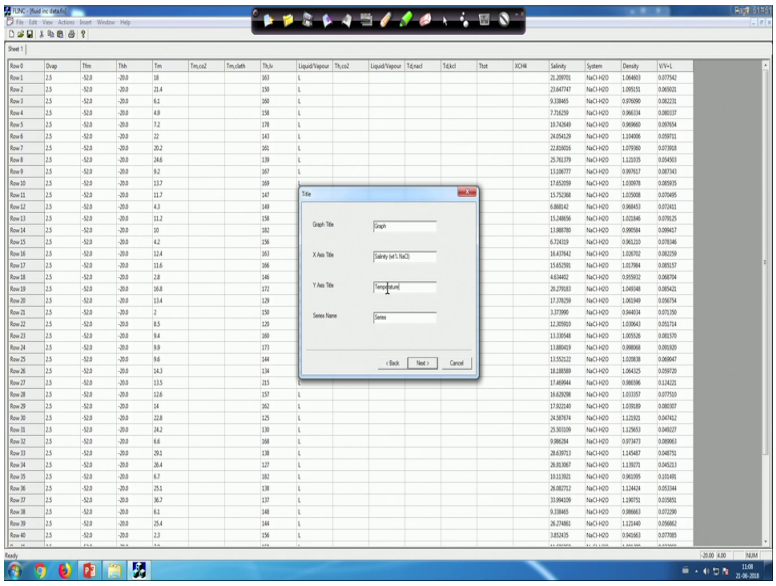

So, this is a situation where I have already filled this box up with data. Yeah another utility of this kind of situation here is that the excel worksheet and general user is very much familiar with working on excel like worksheet and it should have the provision for adding the number of rows because if the fluid inclusion is generated data in hundreds and the there should be scope for entering or giving the input of the entire data set whatever he has been generated. And now, suppose this is the set of data which was generated on all aqueous inclusion and the basic data that was given is the temperature of melting of ice, temperature of liquid vapor homogenization, all homogenization to liquid and then we could see that I have just for the sake of demonstration given the same value of diameter a vapor from face that is measured at 25 degree Celsius and the temperature of fast melting temperature of hydro halite melting and which is are not taken into consideration here.

So, suppose for example, somebody wants to you want to draw a histogram. So, it could be so, which among these are the when it takes into account the plotting of this data, it could be any of the input parameter as well as the output. For example, a temperature of homogenization is an input parameter in densities and output parameter, one can always take the data for plotting of I any of them. Say for example, I will choose a temperature of homogenization T H L V to plot a histogram.

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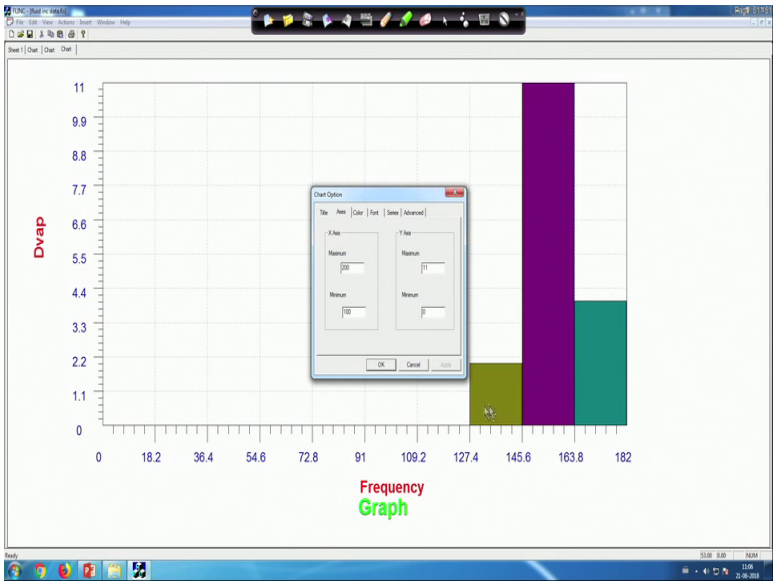

And so, I can I can get the and these are the essentially editable; I just put the range between 100 and 200.

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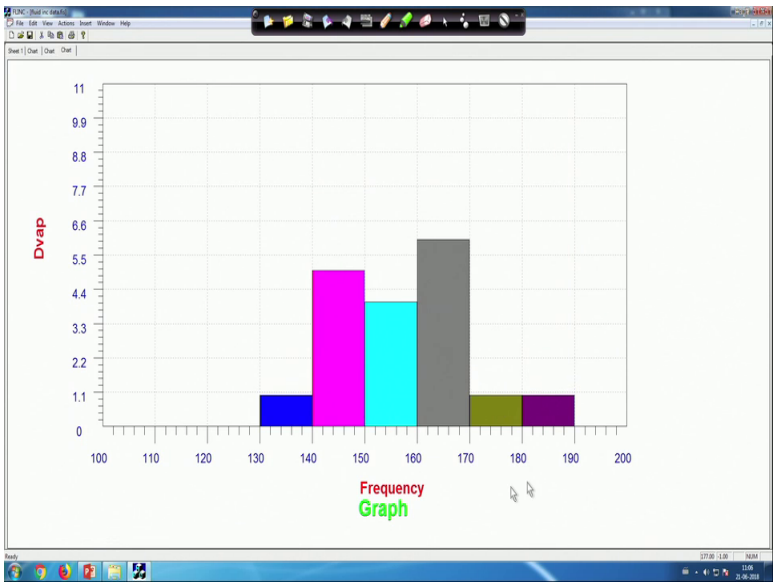

And see class interval is chosen by it is own with given the logic for the development of the taking the particular class interval and then so, this keep a histogram which a fluid inclusion is to like to put it as a final result and presentation of his data. For example, I would like to and let us say that we want to have a scatter graph.

So, in this scatter graph, we it will definitely taken because there are in such kind of packages, the provisions have been made to use more than one worksheet like what happens in an excel worksheet and this takes the x column as the salinity and the y column as the temperature of liquid vapor homogenization and the plots.

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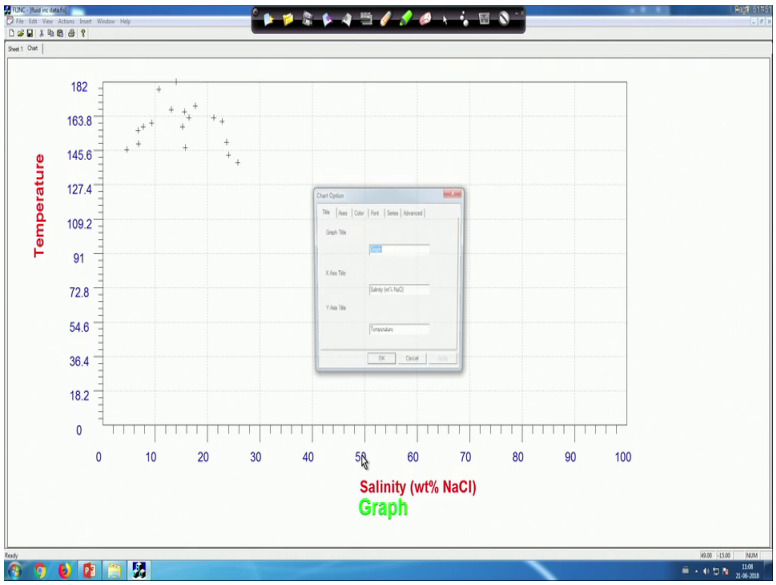

So, we get over data and here we can change the maximum minimum in to get a better picture.

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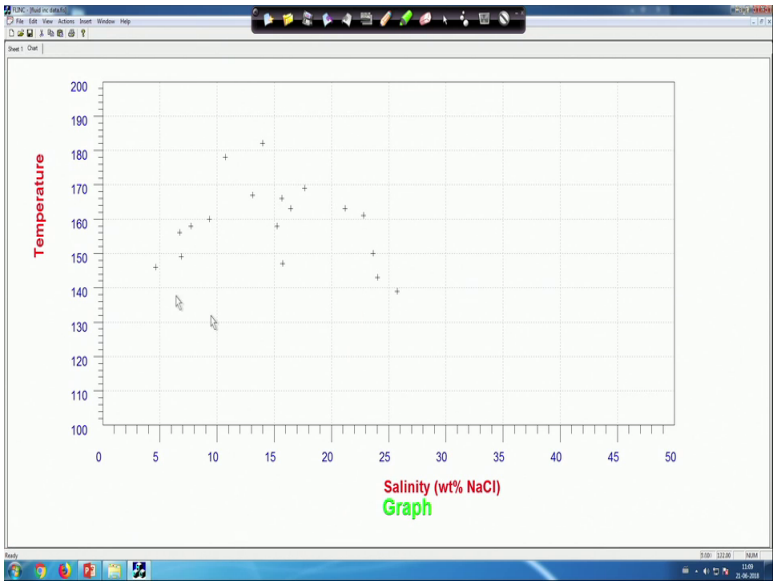

And so here, so this will always haven utility of the editing this particular a graph for putting the legions even more prominent, this data points or any kind of font and any kind of decoration that one would like to do to the graph can be easily done by using the basic utility.

So, this is one example of this is one example of a software packages which will which has been which can be developed for I can be told as a as a platform which will which will be which will take into consideration the need of a fluid inclusion list where on one spreadsheet kind of a workspace, all the all the types of data could be generated, could be entered and then all possible outcome the expected outcome in terms of the isochore, the scotograph, the histograms for all the input and the calculated parameters can be generated.

So, that will that that could be a towards and like it sort of a kind of, if you want a software package which will be a single platform, software packages which will not make one to run around to generate data in one particular output and then taken plot. For example, one can always export the data and then use a scientific graphics software packages like micro cal origin to plot the data and bivariate or kind of histogram are there are possibly are more specialized. But then it will also possible by using the basic functionalities of the available the tools that one can always use to develop such kind of software's for the use of fluid inclusion work. So, we will continue discussing in the next class.

Thank you.