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

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Lecture - 36
Computer Software for Fluid Inclusion Data

Welcome to today's lecture and the last module of the lecture series on Fluid Inclusions in Minerals. We have browse through or we have kind of got an overview of Fluid Inclusions. There different types diversity in the host minerals, in through in diverse type of geological environments. And now we will discuss something that we have planned to that the need of the use of Computer programs and Software's for the analysis of the Fluid Inclusion Data.

The raw micro thermometric data that we acquire from our heating freezing experiments and how to present of their presentation of the data in different forms as we have seen before like histograms by bivariate plots and the isochors. And the procedure calculation procedure involved in calculating the density of fluids; sometimes the mixtures of water with other gaseous species.

The discussion in this particular module will be more general other than any rigorous involving any rigorous formulation and mathematics or even not going into any of the fundamentals of computer programming as such. But the thing is that actually when we say computer modeling. It is not that very appropriate to the use of computer programs or software in fluid inclusion work.

Because it involves only the calculation of certain parameters from the row micro thermometric data and most of the time it most of the cases it boils down to something like formula translation. Because during the course of our discussion we discuss we mentioned or we saw the formulations different types of empirical equations or which we call them is a equation of states.

They were developed for the calculation of the volumetric properties of inclusion fluids at different temperature conditions; different for aqueous inclusions or aqueous carbonic inclusion. The salinity of the aqueous phase and the density of the carbonic component

and then when they homogenized to a total. homogenization. How to calculate their density in isochors?

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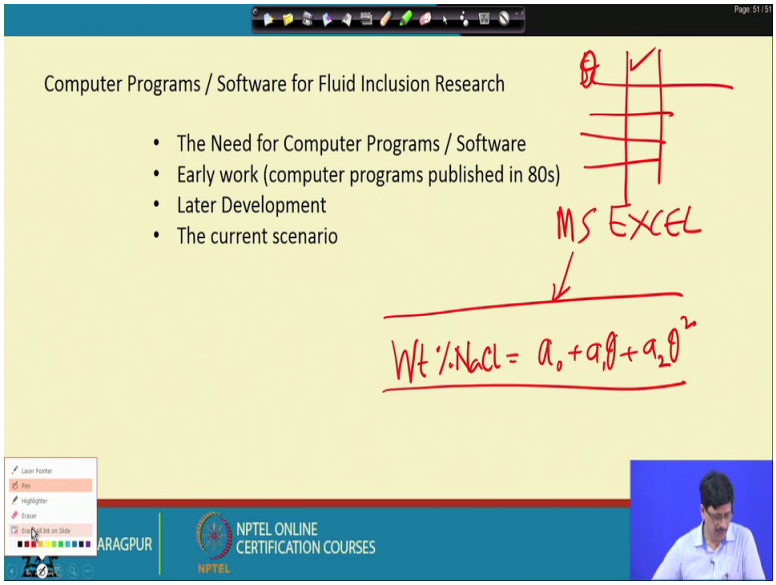

So, this formulations have actually been developed by the by rigorous procedures of theory, as well as empirical observations and sometimes like the discussion which we made on the quantified at least quorum type of equations. Their essentially can be called as a semi empirical in nature by considering certain theoretical aspects of interaction the molecules at high different pressure and temperature conditions, plus what exactly we have come from observations or the experimental measurements of volumetric properties. And then through some analysis like regression type of analysis or different types of mathematical techniques which are used to finally, formulate such equations which will be directly used usable for volumetric properties calculation for fluid inclusion they whatever we get from micro thermometry.

So, the first point that the need for a computer program or a software comes, when because these days because if you take the simple example of where we term where we. So, the for example, weight percent NaCl equivalent from freezing point depression data we see simply that weight percent of NaCl is just equal to some parameter a 0 plus a 1 into theta which is that depression of the freezing point from 0 plus maybe a 2 theta square.

So, when this is a very simple equation to calculate the salinity of as aqueous inclusion where the freezing point depression data is available. Now the thing is that we measure the inclusions in large numbers and calculating them by hand will be time consuming and error from. But then these days it is very simple even if we use kind of an excel Microsoft excel worksheet. They are also we can for any particular field on the,which we call as a cell. We can write the formula and this formula will be very simple formula to put.

So, that when on one column when we give our salinity data sorry the depression in freezing point data theta and for this particular column you just put the formula bar that it will just convert this depression in freezing point to salinity. Then just to the click of mouse will get the data for salinity. And so, but then when it comes to a situation where we have to calculate the density of an aqueous fluid from temperature of homogenization and salinity. There it is a 10, 12 14 coefficient non-linear regression equation and that will be possibly not that very easy to put in a in excel sheet and do this thing very easily.

So, in that case there is a need that we write a computer program, and then run the program and give the input values as our temperature of homogenization and salinity and then get the density values. And also the formula that we have seen for calculation of the d p d t slope which is a function of salinity and the temperature of homogenization and sanity we can also calculate the slope. So, the need for a computer program arises because of the length of the calculation they rigor of the calculation procedure involved and the amount of micro thermometric data the quantity of the micro thermometric data that we have generated which may be in 100 or 1000.

So, then there was a need and in that old older days; when there was no much of facilities where available like what I am talking about the Microsoft excel launch which is a development which came much later compared to when in the 70's or 80's. When such kind of a fluid inclusion is need needed to analyses data or processes data in the form of the final presentable form. So, the need was very much there to so there were many people.

So, in the early stages there were many workers of fluid inclusions; who were writing small Fortran or the small programs in high level programming languages like basic or

Fortran. If someone looks at if someone looks at the John Donne which actually publishes computer.

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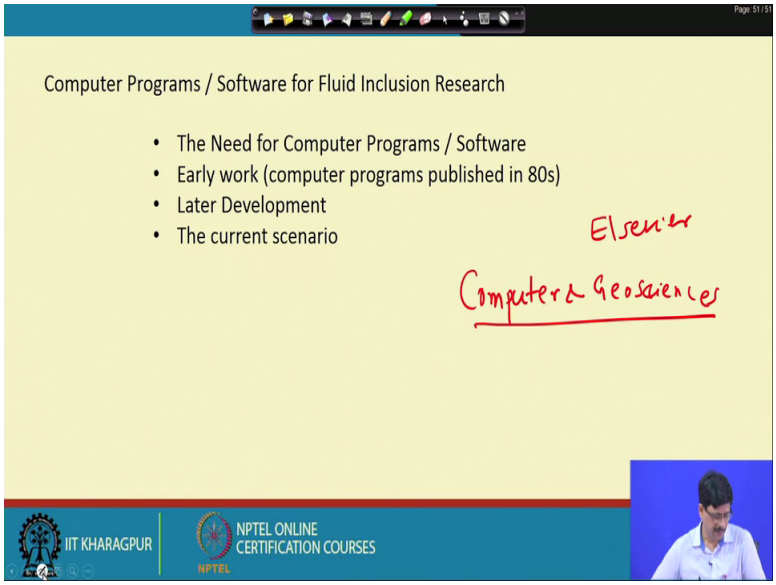

The Computer and Geosciences journal; which is published on Elsevier. If the if someone browses the content of this particular journal the owned archives, one will learn one will see a lot many such small I mean such Fortran or basic programs which we are used to get published by various authors and different points of time. I am not giving an exhaustive list of them. It is at essentially not very relevant here, but the only problem was that when there was a there was a code in high level programming language like basic or FORTRAN was written or given by somebody.

Than one need to have a platform like a if a compiler and where you will run the program executive program and get the results which was also not that very easy in the earlier days. Then what actually happened is the later development. So, it was much easier so those kind of programs which were written in high level programming languages like Fortran or basic. Those programs where essentially what one can say that they were non means these days when any when this computer is available to anybody at everybody.

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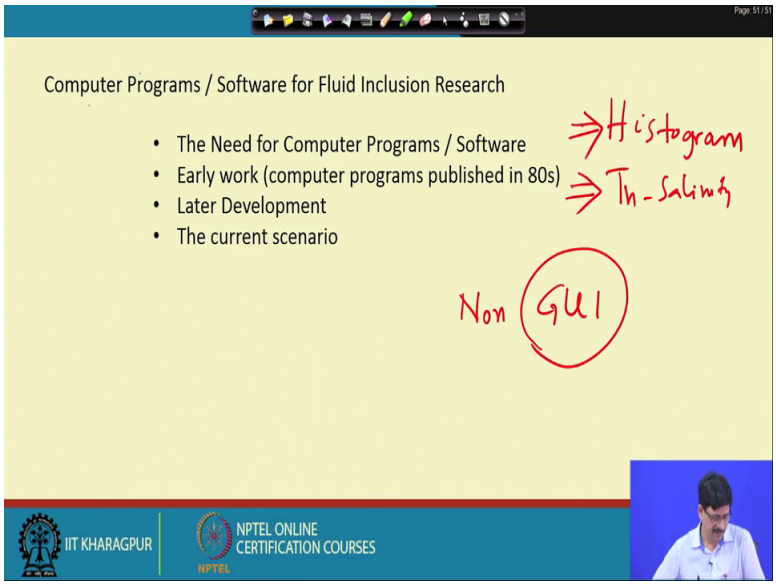

And this the operating system windows operating system that we use and they are so many so much a graphical user interface based that we simply just click of the mouse on the button, we get many of the jobs done. Like menu bars, dialogue boxes, windows all this kind of thing have become so many user friendly these days, which was not there previously.

So, most of these programs which used to be written in high level programming languages; like while I am talking about they were all they were based on non graphical user interface based. Because one is to get the put give the input in terms of either from the counselor form enough in the form of a file. And then also get the output in the form of number, and then there was a need that whatever data we get because if for a fluid inclusionist to present is data. It to look at the statistics of either a salinity distribution or a temperature density etcetera, we need to first plot them on a histogram to look at the fluid characteristic or assess the fluid characteristics or we need to plot them on the fluid evolution diagram which our paired or T h salinity or diagrams or and then; however, the isochors.

So, there was so whatever used to come is a output from this kind of programs they have also again to be taken to a whatever graphics utility programs are available they have to be taken there in plot do the plotting. So, it was always necessary that graphical user interface based program we developed and with a windows Microsoft windows coming

to the main operating system for the desktop computers a personal computers. It become became easy and also it gives people the scope for development of a graphical user interface base put. So, in that situation we I will discuss a little bit about them later.

And so sense sensor were stick to if we so then the later development were all on based on the right developing computer software which you run on which will be essentially graphical user interface paste and to run on windows type of environment, which will become much user friendly for users to use. And then we will look at the current scenario and discuss what is actually available. So, this discussion will be more general and where as the assignments for this particular module we based on some hands on calculation exercise which will be given to you in the course of this lecture.

Now if we if we talk about modeling, so actually so where modeling is essential or useful. In case of fluid intrusion data analysis and presentation as I said that it just needs to be something like formula translation whatever available formulations are there. They need to be put in the from of computer code either on a non graphical or a graphical user interface which will see them and can do the job.

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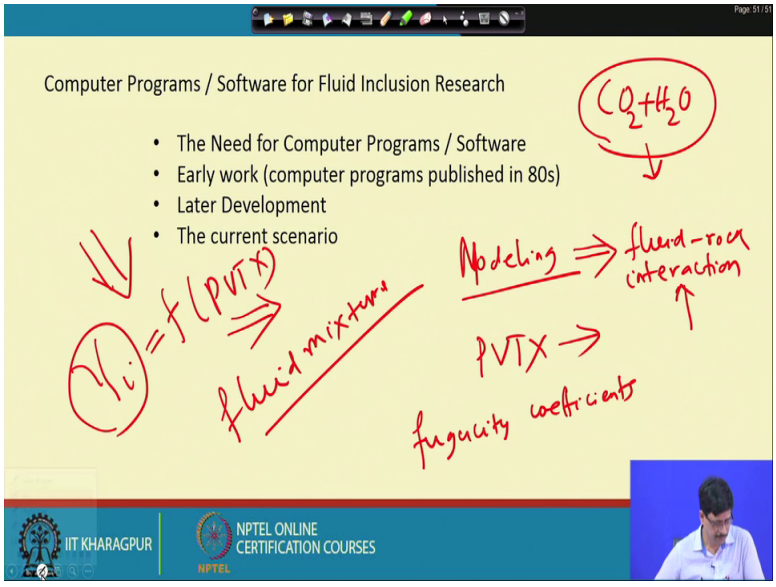

But the modeling was exercise the computer modeling or the modeling exercise, what actually we mean? They are more useful for quantification of the fluid rock interaction. In fact, most of the study of the phase equilibrium on the fluid mixtures whether it is only water plus electrolyte or water plus gaseous volatile species like carbon dioxide

methane and the electrolytes. The basic idea of development of this P V T X relationship is essentially targeted towards quantification of this fluid rock interaction process. Because the fluid rock interaction process that is taking place. We if we write any whether this on a surface processor any sub surface phase or deep deeper are processes. It essentially interaction of fluid rock whether its ore forming environment or metamorphism of different grades that is taking place in the subsurface.

So, these interactions whenever it involves a fluid phase. So, the fluid phase means it is a fluid mixture. So, any reaction that someone writes involving minerals and if it happens to involve a fluid phase. Then it will always necessary to compute the fugacity coefficients of the component species in a mixture. Say for example, we have a mixture of Co2 plus H2O it is an simple system like Co2 H2O if it is a mixture of Co2 H2O. Then we need to compute the fugacity coefficient of carbon dioxide and water independently. So, that we could calculate any reaction equilibria which involves a fluid phase and that fluid phase is not a pure fluid phase, but a, but a mixture.

So, now the situation is that in case of this fluid like the one which we were talking about the component. the fugacity coefficient of this component; so, this each component species if I put it as kind of gamma I. So, I standing for the species like carbon dioxide or water this is a very intricate function of the P V T X relationship of this particular fluid.

So, this fugacity coefficient term in order to be computed it can only come from the P V T X once the P V T X relationship is established then only it will be possible through standard formulations and through use of thermodynamics to calculate the a fugacity coefficient which is a important parameter for quantification of any fluid rock interaction process where there is a fluid phase involved and that. So, once this P V T X relationship which is formulated it is also is useful for volumetric property for the calculation of the volumetric property of the fluid inclusion.

So, since fluid inclusions are being used is one where they tool. So, fluid inclusion fluid rock interaction in the formalism that we are using in a fluid rock interaction they are very much related to each other. So, it is always we can get a clear picture only when we see them together, but we do not have much of scope discussing much of the rigorous exercise involving the calculation of the fugacity coefficient of gaseous species, but then the as it. So, the use of actually a computer modeling is essential whenever we are doing

some or development of any of the existing formulations. Say for example, if we have our situation is that we suppose we are talking about a only are aqueous fluid.

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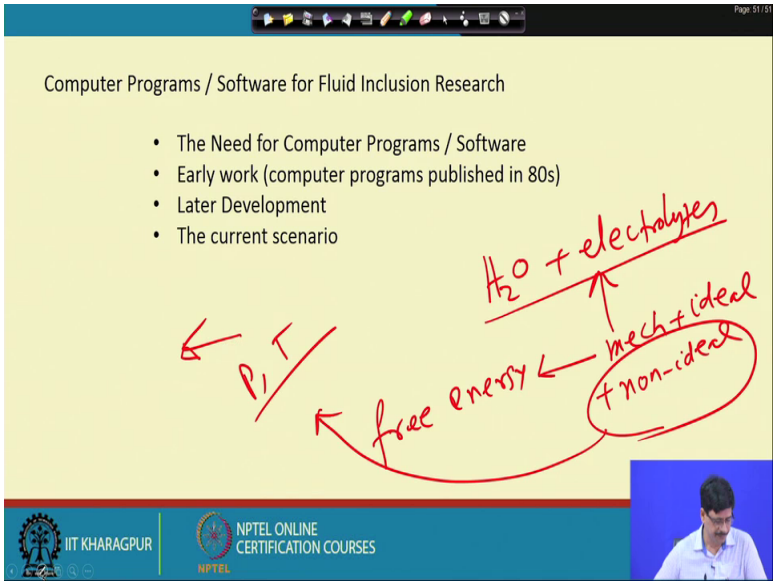

So, that aqueous fluid is water, plus electrolytes this electrolytes our may be the chlorides or any other an ionic species So, here also when we talk about the P V T X relationship this P V T X relationship is also coming into picture for example, we want to when we quantify a fluid rock interaction process involving a aqueous phase which is a fluid. So, there we also know that the way we can express the total free energy which is a which is contributed by the component from the where its it is a solution and as we deal with crystal and solution we also can look at this aqueous solution here in the much the same way, but in a different type of formalism or different logics is applied to that will come from a mechanical mixture component it will come then from a ideal contribution and non ideal contribution.

So, we are mostly so as for as the modeling part this concept is always to account for the non ideality and the parameters that would be contributing to the non ideal behavior of this particular fluid mixture. It is a particular fluid and this non ideality in case of an aqueous electrolyte would be depending on lots of long range and short range interaction parameters of this aqueous charge as well as the aqueous neutral species that represent at different pressure and temperature and conditions.

So, the computer modeling actually is applied to whenever we are looking at them and then trying to improve upon the activity composition relationships in such kind of fluid mixtures. And we can ultimate objective of a applying it to fluid rock interaction processes in a better way to better quantify and also as at the same time a refined P V T X relationship in this kind of situation is also helping us to accurately more accurately calculate the volumetric property like the density and the isochors. As I told you that even that at this particular point of time evens a systems very simple systems like water NaCl system it still being revisited.

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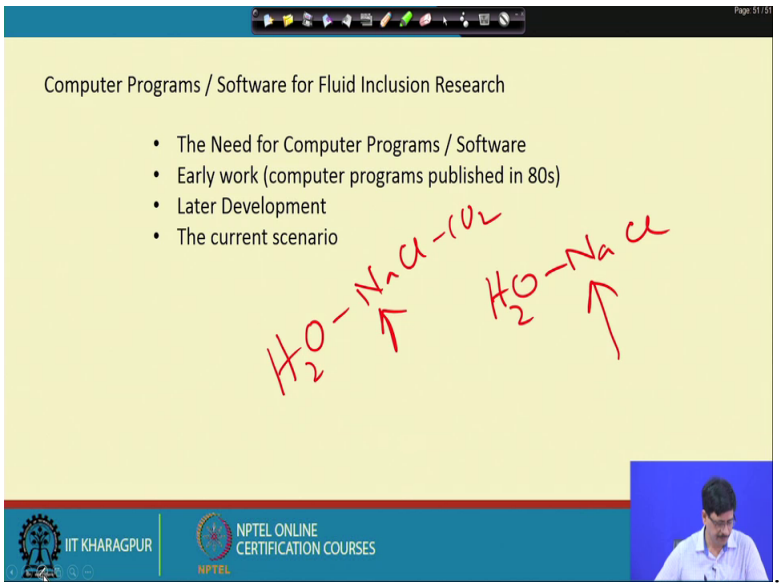

Ah with two for its more rigorous analysis of the phase relations and the invisibility region or whether at all there is invisibility in this particular fluid. And even till today also this particular system is being revisited and also systems like H2O NaCl CO2 it still one of the most widely studied system. But as at the a full have completely I mean a formulation which will be accurately applicable to all pressure temperature conditions pertaining to many types of diverse type of our processes is yet to emerge for this particular system. Because it has been a difficult system and experimental data for this particular system has not that been much.

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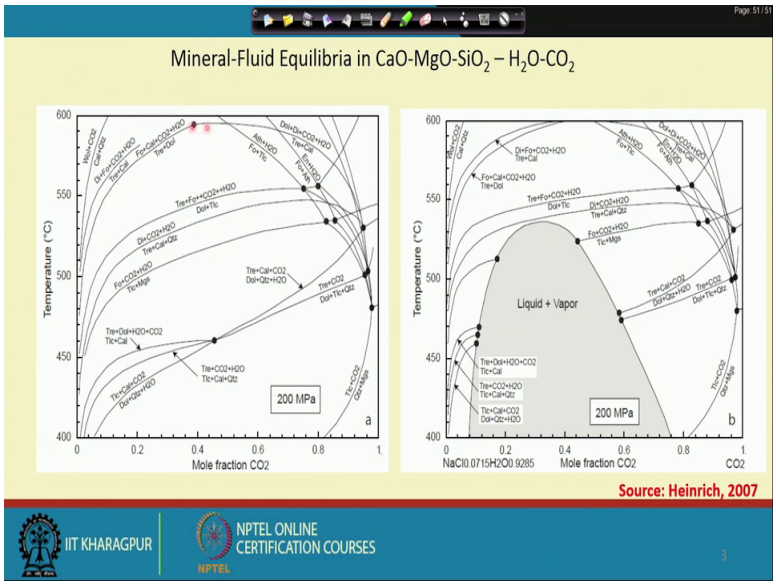

To give you just an example what I discussed that the fluid rock is the computer modeling is used in actually working or the P V T X relationships form that in turn the non ideal parameter in the fluid mixtures to be were to be quantified. And the react suppose for example, this I am showing the just to demonstrate their; suppose there is a reaction dolomite plus talc giving raise to tremolite, forsterite, carbon dioxide and water. So, you could see that it is a fluid mixture that is associated with this particular reaction.

So, this reaction topology this reaction boundary will very much depend on what is the composition of the fluid in terms of carbon its mole fraction of carbon dioxide. And water and not only that the reaction boundary will very much depend on the accurate calculation of the fugacity coefficient of both; this water and carbon dioxide and which needs to have a very complete formulation of the P V T X relationships and that is how it is related.

So, and that is the part where I rigorous computer modeling involving the analysis of the experimental data or some theoretical considerations. And then such kind of quantification will be more possible and here just to show that if the it is showing as a pure carbon dioxide system fluid where the few carbon dioxide and water here the carbon dioxide and water is charge with little bit of sodium chloride. This one is 0.0715 mole fraction. Which gives rise to any visible region and because of that in (Refer Time: 24:01) visible region the topology of the reaction boundaries and the invariant points are

also becoming are also changing. So, these just for the sake of example, not just to make you feel that what exactly when the computer modeling is so many of the programs that we are seeing.

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For example, in I will just briefly go through some of the things that later development in the computer program or software for fluid inclusion data and ok.

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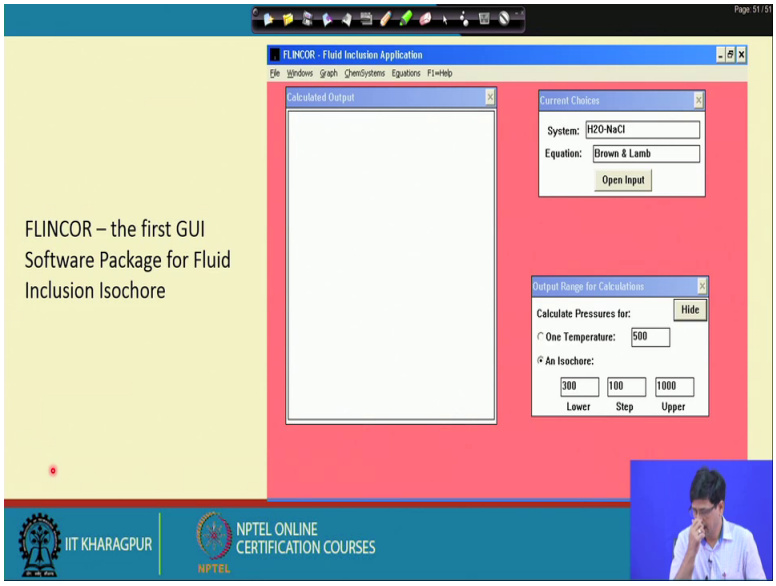

So, when just about the time when this non graphical user interface computer course where b[came getting for these two for use of fluid inclusion. Fluid inclusion is to

process the data and for volumetric calculation for density and isochore. Right about the same time with Microsoft windows coming this particular package the FLINCOR was published in about 1989 by Fill Brown from University Wisconsin. That was a very popular software package that was there the time for fluid inclusion is almost everybody was using this particular software package I am just giving one example because these days it is not actually comfortable with the later versions of the windows operating system.

But this gives some inside from idea is to what how the packages could be developed to how it was developed what was the form of the utility. So, this package was actually for mainly targeted for isochore calculation. So, that is why it was named as FLINCOR so fluid inclusion isochore and this was like working under a graphical user interface where there could be windows there are dialogue boxes where editable boxes where they could appear. And people could into a give their input data and get the calculations done. Just for example, it say a case in which H2O NaCl one through just a system that his inclusion belongs to.

So, when the micro thermometric data at acquisition is over, the user is to specify that what system that particular inclusion fluid belongs to gives the choice and then she was giving a given a drop down menu with choices from many formulations that as available at the time to choose one of them. And then give open an input box where it could give either freezing point depression or halite dissolution temperature or molality or weight percent n a c l or mole fraction.

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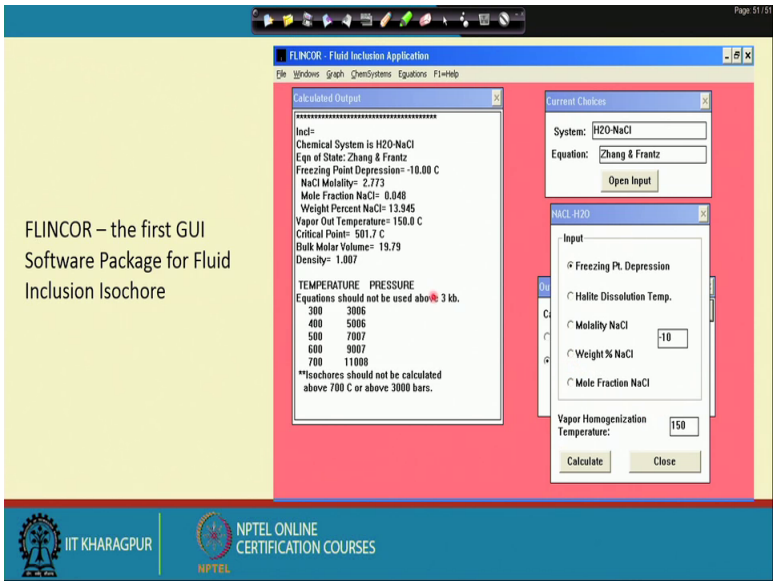

So, this parameters need to be even calculated a one may not be having readily available. So, it is as it is shown that suppose a minus 10 a freezing point depression is given, and the homogenization of temperature was given also specified in a different box. And on taking the calculate button one gets data on the for the particular inclusion. The salinity the density data are calculated in display along with the isochors which you are calculated from a particular temperature range.

So, those formulations there they were actually formula translation from the existing formulations at that time. Suppose the particular formulation was only applicable in a range of 300 to 700 degree Celsius. Then the one in which to come this isochore should not be calculated above 700 degree centigrade or 3000 bars a depending on the formulation of the proposed by the authors like for example, what is written here.

So, the limitation was that so you did not have any. So, no only at one particular time only one inclusion data could be processed and what was coming is the display as the isochore for the pressure at any corresponding temperature interval as because they were distributed in the executable code. So, whatever interval 300 to 700 degree Celsius with 100 degree Celsius interval was kind of by default and this data has to be taken and exported to some other kind of graphic software to plot the isochore.

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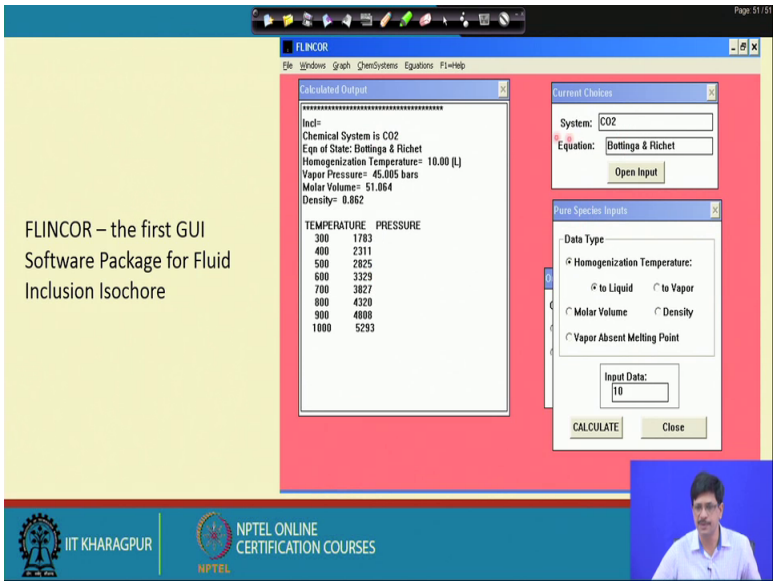

Similarly, the examples are like this is for pure CO2 and similarly whatever was the formulations available at that time for CO2 has to be chosen by the user.

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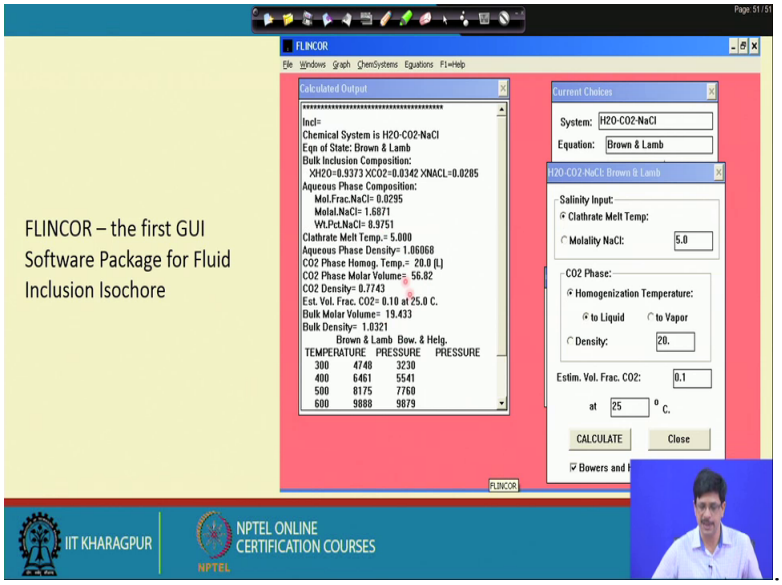

And the calculations will be displayed and the isochore is to isochore used to be displayed.

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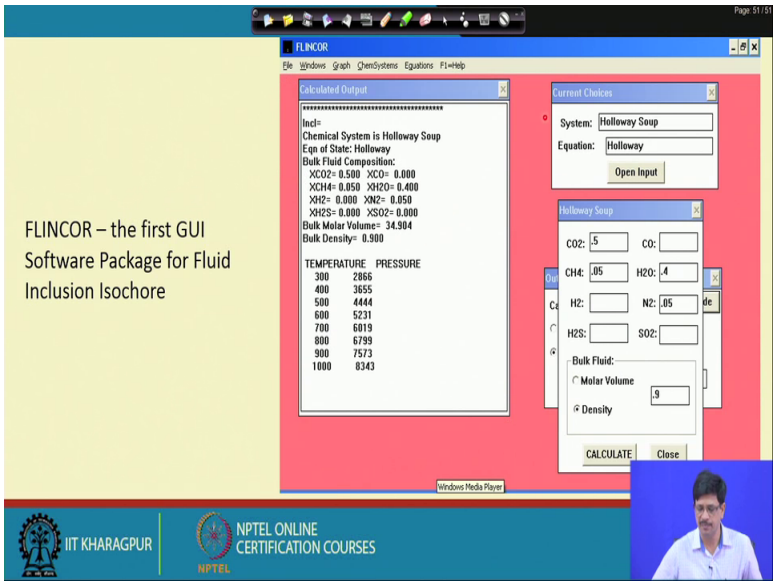

So, this is what as the many systems that are available with the time like for methane.

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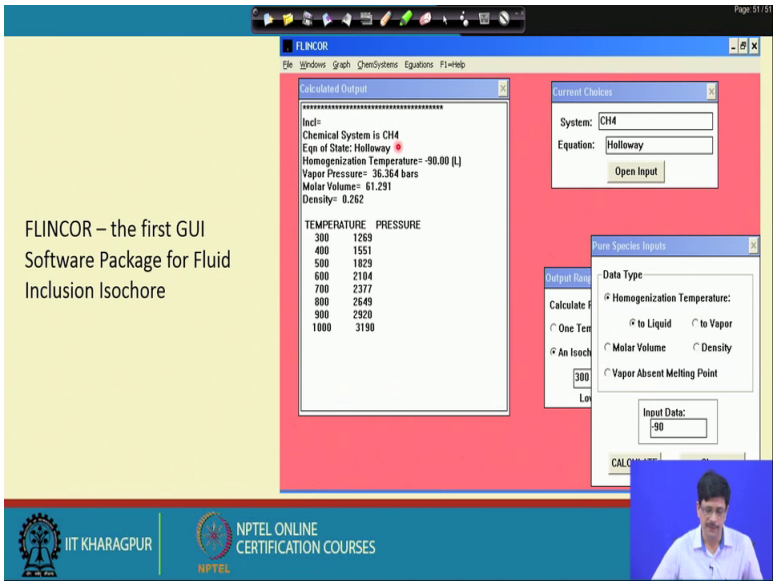

For a fluid mixture like carbon dioxide methane hydrogen H2S CO H2O and to SO2 and there were some formulations which are available which could calculate the P V T X relationship in such kind of a complex fluid mixture and the isochors to be displayed. And again let us to be copied down and then taken to a particular any other particular software where the graph could be plotted.

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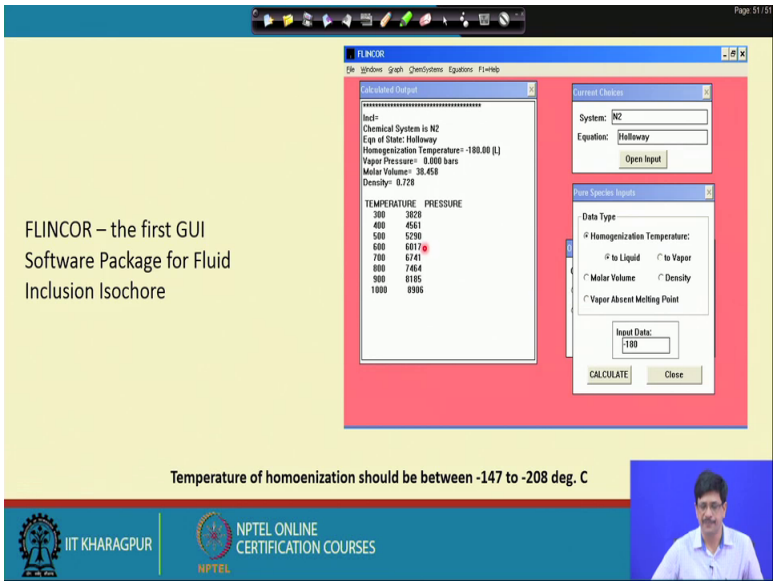

So, it was not this is an example of pure nitrogen. here this only the warning message one could read that it is, temperature of homogenization should be between 1 minus 147 to minus 208 degree Celsius.

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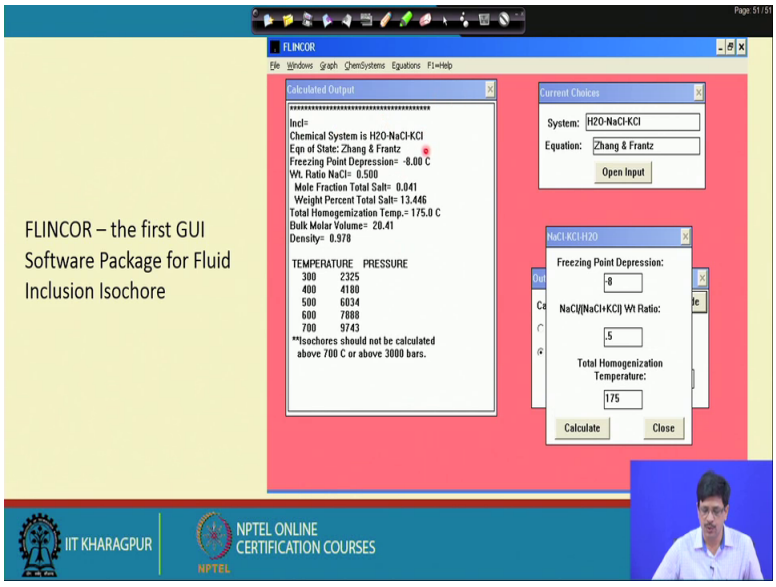

And the, it was for H2O NaCl and KCl the kind of formulations which you also discussed.

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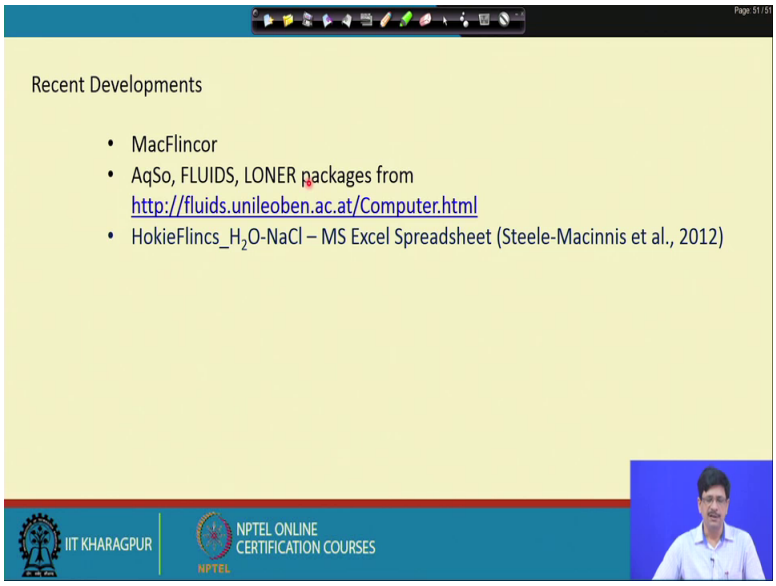

So, now, this was again this limitation not withstanding these programs written in c programming language in and we distributed. And the only situation was that the software's where available they were to be procured and to be used. So, wherever people we are not able to procure that software or used it with their machines. They used to depend on writing their own programs again in the same way, formula translation and then process the data. So, will continue discussing on this in the next class.

Thank you.